

RAINFALL-RUNOFF MODEL CALIBRATION USING
EXPERIMENTAL DESIGNS AND RESPONSE
SURFACE METHODOLOGY

CENTRE FOR NEWFOUNDLAND STUDIES

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**RAINFALL-RUNOFF MODEL CALIBRATION
USING EXPERIMENTAL DESIGNS AND
RESPONSE SURFACE METHODOLOGY**

By

©HERI SULISTIYONO

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Abstract

Rainfall-runoff models used for hydrological modelling usually involve many parameters that must be calibrated using observed rainfall and runoff data before they can be used for any water resources study. Traditionally, calibrations of these models are done using a trial and error approach or by using numerical optimisation methods, neither of which is entirely satisfactory. In this thesis, a calibration based on Statistical Experimental Designs and Response Surface Methodology is presented. This method integrates statistical experimental designs, regression modelling techniques, and optimisation methods in the calibration process. This method can effectively select the parameters and indicates their interactions that will significantly affect the response variable, which in this case is a goodness-of-fit criterion. The method also determines the optimal values of the parameters that should be used in the model to produce the best fit of calculated runoff amounts to observed runoff amounts. Full factorial and fractional factorial designs and two popular response-surface designs: central composite (CCD) and Box-Behnken were compared.

Mock's rainfall-runoff model, a popular model for irrigation planning in Indonesia will be used to illustrate the proposed methodology. It has six parameters to be calibrated from observed monthly rainfall and runoff data. The results of the proposed methodology of calibrating the six parameters of the

Mock model will be compared to those already obtained previously using the trial and error method. Observed rainfall-runoff and evapotranspiration data from 1973 – 1976 for the Babak River Basin in Lombok, Indonesia will be used in the calibration of the model. Data for 1977 and 1978 will be used for verification of the model.

The results showed that the proposed methodology gave a better understanding of how the parameters interact with each other, is more systematic, and the optimised values gave a better fit of computed and observed runoffs.

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List of Symbols

Symbols

Θ_{l+1} = New point;

Θ_l = Initial point;

(1) = The response of the process when all factors are set at the low level;

$\nabla \Theta_l$ = The function gradient matrix at the initial point;

ΣE = Absolute Sum of Error;

$\Sigma(SS_{\text{parameters}})$ = Summation of all sum of squares of parameter-effects;

$\Sigma(\text{response}^2)$ = Summation of all responses of the experiments;

α = Axial distance;

β = Coefficients of polynomial models;

ΔV_n = Monthly change of storage volume;

ϵ = Experimental errors;

η = Hypothetical observed true values;

ρ = Distance of moving;

A = The Matrix of moving direction from Θ_l to Θ_{l+1} ;

A = Single parameter A = The parameter of coefficient of impermeable layer;

A² = Quadratic parameter A = The parameter of coefficient of impermeable layer;

AB = Interaction between parameters A and B;

AC = Interaction between parameters A and C;

- AD = Interaction between parameters A and D;
- AE = Interaction between parameters A and E;
- AF = Interaction between parameters A and F;
- B = Single parameter B = The parameter of initial storage value;
- B^2 = Quadratic parameter B = The quadratic parameter of initial storage value;
- BC = Interaction between parameters B and C;
- BD = Interaction between parameters B and D;
- BE = Interaction between parameters B and E;
- BF = Interaction between parameters B and F;
- C = The number of additional points;
- C^* = The central value of parameter;
- C = Single parameter C = The parameter of coefficient of infiltration;
- C^2 = Quadratic parameter C = The quadratic parameter of coefficient of infiltration;
- CD = Interaction between parameters C and D;
- CE = Interaction between parameters C and E;
- CF = Interaction between parameters C and F;
- COI = The coefficient of infiltration;
- Contrast A = Contrast value of parameter A;
- D = Single parameter D = The parameter of coefficient of recession;
- D^2 = Quadratic parameter D = The quadratic parameter of coefficient of recession;

- DE = Interaction between parameters D and E;
- DF = Interaction between parameters D and F;
- D_v = The Deviation of the Runoff Volume;
- E = Single parameter E = The parameter of soil moisture capacity;
- E^2 = Quadratic parameter E = The quadratic parameter of soil moisture capacity;
- EF = Interaction between parameters E and F;
- Ea = Effective evapotranspiration;
- Effect A= Effect value of parameter A;
- F = Number of factorial points = 2^k ;
- F = Single parameter F = The parameter of initial soil moisture;
- F^2 = Quadratic parameter F = The quadratic parameter of initial soil moisture;
- F_0 = Value of calculated F- test;
- $F\text{-ratio}_c$ = The calculated F-ratio of curvature;
- H^* = The highest value of parameter;
- I = The infiltration rate;
- IMLA = percentage of impermeable layer;
- K = monthly coefficient of recession;
- L^* = The lowest value of parameter;
- M = $(k-1) \rightarrow k$ is the number of parameters;
- MS = Mean of squares of parameter-effects;
- MS_c = Mean of squares of curvature;

MS_E = Mean of squares of error;
 MS_P = Mean squares of parameter;
 P = Probability;
 Pr = Amount of monthly rainfall (precipitation);
 Q_o = Observed monthly river flows;
 $\overline{Q_o}$ = Mean of observed monthly river flows;
 Q_s = Simulated monthly river flows;
 R^2 = Nash Sutcliffe Coefficient;
 RO = Amount of catchment runoff;
 RME = Ratio of Mean Error;
 SMC = soil moisture capacity;
 SM_o = and initial soil moisture;
 SS = Sum of squares of parameter-effects;
 SS_A = Sum of squares of parameter A;
 SS_c = Sum of squares of curvature;
 SS_e = Sum of squares of error;
 SS_{total} = Sum of squares of the total model;
 V_o = Initial storage value;
 V_{ob} = Observed runoff volume;
 V_s = Simulated runoff volume;
 V_t = Storage volume;
 V_{t-1} = Previous storage volume;
 WS = Water surplus;

- X^* = Target of sum of absolute errors;
- X_i and X_j = Parameters of polynomial models;
- X_k' = Levels of factors;
- X_k = Sum of absolute errors;
- Y = Actual observed true values;
- Y = Process that is affected by factors: A, B, and C;
- a = Response of the process when only factor A is set at the high level;
- a_0, a_1 and a_j = Coefficients of the polynomial;
- ab = Response of the process when factor a and b are set at the high level;
- ac = Response of the process when factor a and c are set at the high level;
- bc = Response of the process when factor b and c are set at the high level;
- abc = Response of the process when factor a, b, and c are set at the high level;
- b = Response of the process when only factor B is set at the high level;
- bf = Amount of monthly baseflow;
- c = Response of the process when only factor C is set at the high level;
- dro = Amount of direct runoff;
- df = Degree of freedom of parameter-effects;
- df_A = Degree of freedom of parameter-effect A;
- df_B = Degree of freedom of parameter-effect B;

df_{AB} = Degree of freedom of interaction-effect AB;
 df_c = Degrees of freedom of curvature;
 $exp_1, 2, \dots$ = Experiments number 1, number 2, ...;
 $h(X, \epsilon)$ = Response surface objective function;
 h_m = Measured system response;
 it = I = Infiltration in the particular month;
 k = Number of model parameters;
 n = Required number of experiments;
 n_c = Number of additional replicates of central point;
 n_F = Number of factorial design points;
 p = Number of possible levels for parameter A;
 q = Number of possible levels for parameter B;
 r_{crit} = Critical value of correlation coefficient;
 $storm$ = Amount of storm runoff;
 y = Response;
 x = Parameters;
 \bar{y}_F = Average observations of factorial designs;
 \bar{y}_c = Average runs at the central point;

Chapter 1

Introduction

Rainfall-runoff models are computer based conceptual models used for water-resources management purposes. These models normally have many parameters or coefficients that must be calibrated before the model can be used effectively. Hence, the calibration of a rainfall-runoff model is a necessity before it can be used on a particular catchment. This chapter will describe rainfall-runoff models in general, and briefly describe various calibration methods. The objectives and outline of the thesis are also presented in this chapter.

1.1. Rainfall-Runoff Models

Hydrology is the study of water on the earth. It consists of the study of the water resources, observations, management, and elements of the hydrologic cycle: rainfall, evaporation, infiltration, runoff, etc. One of the main concerns of hydrologists is the study of the water balance in a river basin. Understanding the water balance allows for better management of the water resources available in the basin. A water balance study is basically an accounting procedure to quantify the amount of water that is entering the basin from the atmosphere in the form of precipitation, and the amount of water that is leaving the basin in the form of runoff, infiltration, and evapotranspiration. Hence, from a study of the water

balance over a long period record, one can determine if a persistent shortage of water or a surplus of water is present. One can then determine how the available water should be allocated for water supply, irrigation, hydropower, etc.

The characteristic measurements of runoffs from catchments are very complex. Over the last few years, studies about runoffs have become increasingly important to the community because of the increase in demand for water. Therefore, hydrologists must investigate the availability of runoff in river and other water systems to see whether the needs of the community can be met. When long periods of record of rainfall, runoff, evaporation, and other losses are available, the study of the water balance is rather straightforward in that the historical data can be used directly in the accounting process. However, in most situations, especially in a developing country like Indonesia, runoff records are often very short while rainfall records tends to be available for a much longer period. This is because it is easier and cheaper to measure rainfall than runoff. In such situations, it is common for hydrologists to use mathematical models that mimic the hydrological processes of the river basin to generate simulated runoff data based on available rainfall data. Ideally, models that fully replicate the runoff processes should be used. However, it would be impossible to apply a full description because it is very complicated and interrelated. Alternatively, simulation models can be used. These models are based on a collection of principles set out in mathematical formulation that attempt to describe the characteristics of a river basin. These mathematically based hydrologic models are normally called rainfall-runoff models or more accurately, conceptual rainfall-

runoff models. Many such models are available ranging from the very complicated to rather simple ones. Some are discrete event (based on a single rainfall-runoff event) models, while others are continuous events (based on hourly, daily, or monthly data) models. Some of the better known discrete event models are Hydrologic Engineering Center (HEC-1) Model, Runoff Routing Model Hydrograph Synthesis Model, and Storm Water Management Model (SWMM). Some well-known continuous event models include Tank Model, Streamflow Synthesis and Reservoir Regulation (SSARR) Model, Simple Lumped Reservoir Parametric (SLURP) Model, Hydrological Simulation Program – Fortran (HSPF) Model, (Sorooshian and Gupta, 1995). Practically all rainfall-runoff models are in the form of a computer program. Models that are based on hourly or daily data can also be used for flood forecasting purposes.

With the advent of fast modern computers, these computer-based rainfall-runoff models are becoming easier and more convenient to use in practice. These models can be used to generate simulated runoffs for different scenarios of rainfalls, land use changes, etc. in only a matter of minutes on a fast computer.

However, before the chosen model can be effectively used, the model parameters must be properly calibrated. Different models have different number and types of parameters. Two types of model parameters are normally used in rainfall-runoff models: "physical" and "process" (Sorooshian et. al. 1995). Physical parameters are parameters that represent physically measurable properties of the watershed, for example, drainage areas, fractions of the

watershed covered by lakes, surface and stream slopes, etc. Process parameters are parameters that represent indirectly measurable properties of the watershed, for example, effective depths of water, interflow rates, coefficients of infiltration, percolation, soil storage, etc. Mistaking the true value of parameters will lead to incorrect results. As such, these parameters must be properly calibrated with observed rainfall-runoff data so that the parameters can truly represent the rainfall-runoff process of the river basin being modelled.

1.2. Rainfall-Runoff Model Calibration

In hydrology, Sorooshian and Gupta (1995) define calibration as the process by which the parameters of a model are adjusted. Calibration is needed to adjust the model parameters so that the model can produce simulated runoffs that are similar to the observed runoff data.

There are three general methods of model calibration: "*manual*" (see, for example: Liong, 1991; Sorooshian and Gupta 1995), "*numerical*" (see, for example: Sorooshian and Gupta 1995; and Javaheri, 1998), and "*Response Surface Methodology*" (see, for example: Liong and Ibrahim 1991, 1993 and 1995). Manual methods, also called trial and error methods, are commonly used in practice. However, these methods require numerous trials and little guidance is available to optimise the parameters of the model unless the user has extensive experience with the model and river basin. All parameters are treated independently and usually the relationships among parameters are not explicitly

known. The more parameters involved in the model the more difficult it is to determine the correct values of the parameters.

Numerical methods are automatic calibration methods invented to overcome the problems of manual methods (Dawdy and Donnell, 1965). However, researchers are also not satisfied with most numerical methods because they have to develop their own computer programs which are very specific to the model and are very difficult to be modified by new users (Beck and Arnold, 1976; Sorooshian and Gupta, 1983). Building the program is the most difficult part of the work, as the modellers have to spend a great deal of time developing the programs rather than conducting the model calibration itself. In addition, how the parameters are interrelated is also not explicitly known and taken into account in the calibration process.

To overcome some of the difficulties with the above two methods, Liong and Ibrahim (1991, 1993, and 1995) suggested the use of the response surface method, a statistical-mathematical combination method for model calibration. Liong and Ibrahim used this new method to calibrate the eight parameters of the Storm Water Management Model (SWMM) to preserve the response of peak-flows and runoff-volumes from storm data in Singapore. They used the Nash Coefficient (R^2) values as the response for the goodness-of-fit objective-function. Their results showed that the Response Surface Methodology is an effective model-calibration method. It was simpler and more methodical than the manual and numerical methods.

1.3 Thesis Objectives

This thesis will present the use of the Response Surface Methodology for model calibration suggested by Liong and Ibrahim. While the Response Surface Methodology is well documented in statistical applications, its application to rainfall-runoff model calibration is still limited. Many practical issues dealing with the method and transferability of the method to other models need to be addressed.

This thesis has four objectives, all of which are related to the use of the Response Surface Methodology for calibrating a rainfall-runoff model. These objectives are:

1. To calibrate the Mock rainfall-runoff model using the Response Surface Methodology. The Mock model is used as the illustration because it is commonly used in Indonesia especially in irrigation planning (Mock, 1973; Kadarisman, 1993; and Kurniawan, 1994). The Mock model has six parameters that require calibration using observed rainfall and runoff data.
2. To investigate how the parameters of the Mock model are related and interact with one another. Unlike other methods, one of the benefits of the Response Surface Methodology is the ability to analyse the interaction of parameters. It is important to consider the effects of interactions because they contribute to obtaining the global optimum values of the parameters. The Response Surface Methodology applies experimental design methods for this purpose. The results of two types of experimental designs, full factorial and fractional factorial designs, will be compared in selecting the significant parameters and

parameter-interactions to optimise the objective functions. Kadarisman (1993) argued that only using one objective function is not sufficient to analyse the results of calibrations because different objective functions provide different measurements of a specific change of data and parameters. As such three different objective functions will be used in this thesis.

3. To select the optimum parameter values for the Mock model. Two common experimental designs for Response Surface Methodology, Box-Behnken and Central Composite Designs will be compared. The number of required experiments based on the two designs will also be compared.
4. To demonstrate the accuracy of the Response Surface Methodology over the trial and error method. Statistical approaches and verification techniques will be used to compare predicted and observed runoffs based on different scenarios of data availability. The trial and error method is used as the comparison because it is the most common method of model calibration in practice and because an automatic calibration routine is not available for the Mock model at present.

Monthly rainfall, runoff, and evapotranspiration data from 1973 to 1976 for the Babak River basin in Lombok, Indonesia will be used for the model calibration. Data for 1977 and 1978 will be used for verification of the calibrated model. Further information concerning the Babak River basin can be found in Kadarisman (1993).

1.4 Outline of The Thesis

The thesis consists of seven chapters. Chapter 1 introduces the background of rainfall-runoff model calibration, objectives of the research, and outline of the thesis. It also discussed what rainfall-runoff models are, their purpose, and why they need to be calibrated.

Chapter 2 provides a detailed review of model calibration methodology, especially previous application of the Response Surface Methodology for rainfall-runoff modelling.

Chapter 3 describes the orthogonal experimental designs: full 2^k factorial and fractional 2^k factorial designs, as this is the first stage of the Response Surface Methodology. Advantages, disadvantages, and difficulties of the experimental designs are discussed. In addition, three objective functions: Sum of Absolute Differences between the observed and simulated runoffs, $|E|$, Nash Coefficient, R^2 , and Deviation of Runoff Volume, D_v are defined here. The results of goodness-of-fit measures using the three objective functions will be used as the inputs in the response-surface optimisation stage.

Chapter 4 describes the two popular techniques of response surface optimisations: Box-Behnken and Central Composite Designs. In addition, procedures for model verification are presented in this chapter.

Chapter 5 briefly explains how the Mock rainfall-runoff model works. The parameters of the model are described here. The logic of the model is presented using flowcharts.

Chapter 6 discusses the results of experiments, effect estimations, polynomial models, results of optimisations and verifications. In addition, the comparison among the results of manual calibration, Box-Behnken, and Central Composite Designs are presented here.

Chapter 7 presents the conclusions and recommendations for further study.

Chapter 2

Literature Review of Calibration Methods

This chapter provides a general description about model calibration methods that are currently used. Manual Method will be described in Subsection 2.1, followed by Numerical Methods in Subsection 2.2, and then Response Surface Method in Subsection 2.3. The reasons as to why the Response Surface Methodology is advantageous among those methods are also explained in this chapter.

2.1. Manual Method

Engineers and modellers traditionally conduct calibration of hydrologic models, using “*manual calibration methods*” (Soemarto, 1995) commonly known as the “*trial and error methods*” (e.g., Brazil, 1988 and Kadarisman, 1993). While the method is easy to use and simple in concept, the results are not always accurate and satisfactory. Subjectivity, personal experiences, and even luck are very much involved in the calibration process results. In general, modellers have to manually adjust the parameters one by one. The parameters are repeatedly adjusted to obtain a match between simulated and

observed runoffs. The match can be evaluated using graphs and / or goodness-of-fit criteria. In the graphical method, each time a model parameter is adjusted, both simulated and observed runoffs are plotted together in a graph. The graph has typically a vertical scale of runoffs and a horizontal scale of time. Optimum results are achieved if the simulated runoff curves are similar to the observed runoff curves. In the goodness-of-fit analysis method, goodness-of-fit criteria are used as a measure of closeness between simulated and observed runoffs. Commonly used criteria include Sum of Absolute Differences between the observed and simulated runoffs, /E/, Nash Coefficient, R^2 , and Deviation of Runoff Volume, Dv. In the optimisation process, modellers have to minimise the /E/, to maximise the R^2 , and to minimise the Dv. The perfect optimum results are achieved if /E/ is zero, R^2 is one, and Dv is zero.

The manual method usually has no set sequence for adjusting model parameters. Modellers freely choose and make a set sequence of model parameter adjustments unless the modeller is familiar with the special behaviour of the parameters of the model. they can then determine the sequence of the parameters to be adjusted. However, the results are sometimes different when starting with a different parameter. This is because parameter-interaction effects cannot be taken into account in the manual calibration process. Therefore, the results obtained are not the global optimal parameters.

Typical steps required in manual calibration (Kadarisman, 1993) are:

- (1) *Select the possible range of all model parameters.* Every model parameter must have a possible range where the parameter can significantly affect the model output (runoffs). The parameters' ranges should be taken from the basin of interest because all the model parameters indicate the particular characteristics of the basin of interest.
- (2) *Divide each model parameter's range into several levels.* The divisions are at least two levels: the low and the high to find the direction of the optimum. More levels used will produce better results. The main purpose of the range of division is to determine the optimum and the number of peaks in the range. One peak range is called *uni-modal* range and more than one peak is called *multi-modal* range. In the case of *uni-modal* ranges, the optimisation can directly be analysed at around the peak. However, in the case of multi-modal ranges if the optimum of interest is the peak, the optimisation must be tried at around every peak or at around the highest peak.
- (3) *Set all parameters to the lowest level.* As in the preliminary stage of the process, all parameters are set to the lowest level to have a basic value of optimisation.
- (4) *Choose and calculate the objective functions.* The objective functions are goodness-of-fit measures to be described in detail later in Chapter 3. This research deals with three goodness-of-fit objective functions: $/E/$, R^2 , and Dv .

- (5) *Choose one parameter to be adjusted.* The optimisation of the parameters can only be done one by one. As mentioned before, there is no priority in selecting the first parameter to adjust.
- (6) *Set the parameter to the next level of the range and recalculate the objective functions.*
- (7) *Compare the recalculated objective functions to the previous calculation.*
- (8) *Choose the better results of objective function calculations.* The better results replace the previous basic values.
- (9) *Plot and see the match of the simulated and observed runoffs.* The graph is for visually checking the goodness-of-fit.
- (10) *Repeat steps (6) to (10) until the optimum values of objective functions are achieved.* The optimum values of the parameters will be indicated, if the next level of parameters cannot produce better results anymore.
- (11) *Repeat steps (5) to (10) for another parameter to be adjusted.* All parameters must be adjusted to obtain the optimum value of objective function. The calibration exercise is terminated after all parameters are adjusted, although it is not possible to know if the result is really the global optimum value.

Disadvantages of the Manual Methods:

The trial and error method while easy to conduct, is unsatisfactory because:

- (1) This method cannot explain the relationships between the parameter-interactions. It is difficult to adjust those parameters without understanding the effect of parameter-interactions. Sometimes, increasing one parameter while the other parameter is at a low value has a very different effect from when the other parameter is at a high value.
- (2) Adjusting parameters cannot be done all together at the same time. It must be done one by one. This is why the method requires a great deal of time.
- (3) Manual calibration methods cannot achieve the global optimum because of the parameter-interactions.
- (4) It is difficult to know exactly when the process should be terminated because it is difficult to know whether the optimal values of the parameters have been obtained.
- (5) Modellers who are trained and experienced may be able to obtain good results using this calibration method. However, it normally takes a long time for a less experienced person, because there is usually very limited guidance in the calibration process.

In view of the above problems, modellers have developed new methods usually facilitated by the advantages of computers. These methods

are called the "Automatic Calibration" or "Numerical" methods (Dawdy and O'Donnell, 1965 and Nash and Sutcliffe, 1970). The methods are technically the extension of manual calibrations (Sorooshian and Gupta, 1993). The next section describes these methods.

2.2. Numerical Methods

Numerical methods are developed based on numerical measures of goodness-of-fit using mathematical solutions usually facilitated by using advanced computer programs. The numerical measures are normally computed using methods such as Least Squares (Kuczera, 1982), and Maximum Likelihood (Sage and Melsa, 1971. Bard, 1974. Diskin and Simon, 1977. Sorooshian and Dracup, 1980. Sorooshian and Arfi, 1982. Sorooshian and Gupta, 1983) among others. The principles of least squares estimation and the maximum likelihood estimations are not given here but they can be found elsewhere, for example. Devore (1995). The performance of the objective function computation is the main consideration instead of comparing the simulated and observed curves to obtain the optimum result. The results of objective function computations can also be plotted in three-dimensional graphs that can show relationships among every two-parameters of interest and the yields of the process. Modellers can then focus the experiments to the region of interest that is shown in the graph to obtain the optimum.

Numerical methods are normally categorised as belonging to "*Local Search Methods*" or "*Global Search Methods*", (Sorooshian and Gupta, 1983 and 1995). These methods are described next.

Local Search Methods

The methods are designed to efficiently optimise uni-modal functions (Sorooshian and Gupta, 1993). Uni-modal functions are functions that have only one peak or trough. Exercises included in the method (Sorooshian and Gupta, 1995) are:

- (1) *Select a direction to the optimum using surface graphs.* Modellers can easily select the direction to the place of optimum using the surface graph. The surface graphs are built from the objective function plots.
- (2) *Calculate the necessary distance to move.* After finding the direction to the optimum, modellers have to conduct other experiments or trials that are expected to produce improving results of objective functions such as minimising objective functions. The distance to move can be calculated using the methods of steepest ascent or steepest descent (Myers and Montgomery, 1995).
- (3) *Compute the objective function and plot the result.* After getting to the new region of experiments, the new experiments have to be conducted and then the objective function must be recalculated based on the new experiments. The results of objective functions are then plotted on the surface graphs.

(4) *The procedures (1) to (3) are conducted repeatedly to find the optimum result.* Termination of the process is if the results have achieved the optimum. It means that the process cannot improve the values of objective functions anymore.

The methods utilise three operations, reflection, contraction, and expansion (Javaheri, 1998). Javaheri defined a reflection by a reflection coefficient and the points on where the experiments are conducted. An expansion is carried out when a new minimum is produced. However, if the reflection cannot produce a minimum, then a contraction must be conducted. The Local Search Methods can be divided into two classes of strategy: *“Direct Search Optimisation Strategy”* and *“Gradient Optimisation Strategy”* (Sorooshian and Gupta, 1995).

1. Direct Search Optimisation Strategies

The strategy to achieve the optimum relates directly to the value of objective function. It was reported by Sorooshian and Gupta (1995) that many modellers had successfully applied the methods e. g., Rosenbrock (1960), Nelder and Mead (1965), Dawdy and O'Donnell (1965), Pickup (1977), Sorooshian and Arfi (1982) and Sorooshian and Gupta (1983) among others. Typically, the strategy follows the steps (Sorooshian and Gupta, 1993) below:

- (1) *Start from initial point in the graph.* The graph is built from the objective function plots. The initial point of interest can be chosen at any point in the graph. The point represents the value of objective function in the graph. The initial point is called the central point.
- (2) *Select some new points around the central point.* This step is to determine the direction of the optimum.
- (3) *Calculate the appropriate distances to move in that direction.* The methods of steepest ascent or steepest descent (see for the details of the methods, Myers and Montgomery, 1995. Montgomery, 1997) are applied here to calculate the distance. The new experiments based on the distance are conducted.
- (4) *Evaluate the objective function at the new points.* The objective functions are recalculated based on the new experiments.
- (5) *Take the point that improves the value of objective function as the new point replaces the initial point.* Objective functions at all selected points are compared. The point that produces an improvement of objective function is taken as the new central point instead of the previous central point.
- (6) *The procedures (1) to (5) are conducted repeatedly until the optimum result is achieved.* The process is terminated after achieving the optimum result that is indicated by the smallest, largest, or certain values of objective function.

Sorooshian and Gupta (1995) reported that the strategy provides no guidance to choose the best initial point for starting the process. Naturally, the exercises are done forward at all directions around the initial point. After finding the best direction to move the experiment, the values of objective function have to be evaluated. If the new point has an improving value of objective function then the new experiment replaces the previous one and the procedure is repeated. However, if the new point has a worse optimal value of objective function then the distance of moving is reduced. The search terminates after the strategy cannot find improvement in all directions. Javaheri (1998) reported that the strategy provided a good fit between observed and simulated flows as indicated with Nash Coefficient, R^2 values mostly above 0.80. However, Javaheri found that the use of the strategy was not very robust. The successfulness of the strategy depends on the starting location. It, therefore, could sometimes mislead modellers to obtain the global optimal solution because of being trapped in the local optimal region.

2. Gradient Search Optimisation Strategies

The strategies deal with the information of function values and function gradients. The strategies have been applied by Duan et al. (1992). Most gradient strategies are analysed based on the eq. (2.1) (Sorooshian and Gupta, 1995).

$$\Theta_{I+1} = \Theta_I - \rho \cdot \mathbf{A} \cdot \nabla \Theta_I \quad (2.1)$$

where

Θ_{I+1} = New point,

Θ_I = Initial point,

ρ = Distance of moving,

\mathbf{A} = the matrix of moving direction from Θ_I to Θ_{I+1} ,

$\nabla \Theta_I$ = Function gradient matrix at the initial point.

As in the direct strategies, the new point will replace the previous point if the value of Θ_{I+1} can improve the results of optimisation. The strategies will be terminated after finding the improvement is impossible. It is also indicated by the gradient value if it is significantly close to zero. The reason that the local search methods are unsatisfactory is that they cannot detect the appearance of multi-modal functions. The multi-modal functions are the functions that have more than one peak or trough. The method can analyse one peak or trough only. Consequently, the optimum achieved is not the global optimum but the local optimum. Meanwhile, most hydrological cases have multi-modal functions (Sorooshian and Arfi, 1982). Therefore, *"Global Search Methods"* are developed as an improvement of the *"Local Search Methods"*.

Global Search Methods

The methods are designed to optimise multi-modal functions. The approach strategies include the methods of *"Random Search"*, *"Multi-start Algorithms"*, and *"Shuffled Complex Algorithms"* (Sorooshian and Gupta, 1995).

1. Random Strategy

The strategy uses random numbers generated based on probability distribution functions. Mostly used is the uniform distribution (Sorooshian and Gupta, 1995). For the *"Pure Random Search"* strategies, Sorooshian assumes there is no prior knowledge of where the best parameter set exists. All exercises included in the method are purely randomised. therefore, there is no guidance from the previous exercise to the next exercise. It makes the methods inefficient. Latterly, the *"Adaptive Random Search"* strategies are developed to improve the performance of the *"Pure Random Search"*. However, it was reported by Sorooshian and Gupta (1995) that Duan et al (1992) were not satisfied with their results because there was only a 30 % success rate. The method has been applied by Brazil and Krajewski (1987). Typically, the strategies follow (Duan, et al., 1992) as:

- (1) *Choose a focal point.* This point is for the centre of the process of optimisation. It can be the best point obtained in the preliminary process of defining the parameter range. The best point means the point that has for example the smallest value of objective function. Store the set of

parameters that produces the focal point. Name the set of parameters as the focal parameters.

- (2) *Generate a set of N points for the parameters randomly distributed based on the focal parameters.* Sorooshian suggests using uniform or normal distributions. The values of objective function are computed for every point of the set of parameters. Choose the location of the point with the best value of objective function. Store the set of parameters that produces the best point and name them as the new focal parameters.
- (3) *Repeat step (2) based on the new focal parameters.* This repetition will produce a better value of objective function.
- (4) *Compare all the stored points and determine the point with the best value of objective function.* Re-define this point to be the new focal point. Record in which range level this point was found.
- (5) *Repeat steps (2) to (4) until the optimum objective function is found.* The process is terminated when the optimum value of objective function is achieved. The set of parameters that produces the optimum value is set as the calibrated parameters.

2. Multi-Start Algorithms

This is a simple combination method that deals with multiple optima. Here, the failure probability of the problem of interest, which can still be accepted, must be determined first. The strategy is to run n number of trials of a local search method starting from a random initial point to find the minimum

failure probability. The efficiency of any multi-start procedure varies nonlinearly based on the accepted failure probability. According to Sorooshian and Gupta (1995), Duan et al (1992) successfully demonstrated the strategy to a simple hydrologic watershed model. Weaknesses of the methods (Sorooshian and Gupta, 1995) are:

- (1) Results that are more accurate require a large number of random numbers.
- (2) It is influenced by personal decision because it needs an accepted failure probability.
- (3) There is very limited guidance to conduct the optimisation procedures for a new model.
- (4) The relationships between parameters and their interactions are never described.

In general, steps of the process follow the strategy of random search methods. The difference between the multi-start algorithms and the random search methods is the multi-start algorithms starts from all points of possible parameters (Sorooshian and Gupta, 1995).

3. Shuffled Complex Algorithms (SCA)

According to Javaheri (1998), Duan et al. (1992) had concluded that the large number of minor optima was the most probable reason why the previous attempts were not successful. Therefore, the method of Shuffled

Complex Algorithms was developed. This method is based on the notion of sharing information and on concepts drawn from principles of natural watersheds (Sorooshian and Gupta, 1995).

Here, the weight of the complexes is indicated first, then the sample size of interest is calculated. The sample is generated based on a uniform sampling distribution without prior information. The strategy of this method consists of computing a sample size, generating a sample, ranking the points, partitioning into complexes, evolving each complex, shuffling complexes, and checking the convergence (Sorooshian and Gupta, 1995). Measures of the convergence often depend on how the *closeness* of measuring the distance between functions is defined. Another common description of measuring a convergence is, *uniform convergence*, which requires that the maximum value of the absolute errors in the domain is zero (Elden and Koch, 1990). This is stronger than *point-wise convergence* as it requires a uniform rate of convergence at every point in the domain. The other commonly used measure is *convergence in mean* that involves measuring an *average* of a function of the point-wise-error over the domain (Lorenzen and Anderson, 1993). The convergence properties of an algorithm are described by two analytic quantities: convergence *order* and convergence *ratio*. A sequence $\{X_k\}$ is said to converge to X^* if the following equation holds

$$\lim_{k \rightarrow \infty} \|X_k - X^*\| = 0. \quad (2.2)$$

where:

X_k = Sum of absolute errors.

X^* = Target of sum of absolute errors.

Convergence properties of most minimisation algorithms are analysed through their application to convex *quadratic functions*, for example: *second order polynomial models*. General functions can be approximated by a quadratic convex function in the neighbourhood of their local minima. The convergence properties obtained for convex quadratic functions are usually applied locally to general functions. However, such generalisations do not guarantee good behaviour in practice on complex, large-scale functions.

The Shuffled Complex Algorithms procedures are complex, iterative, and require conditional decisions. The conditional decision of every modeller is different which is why each modeller has to write his or her own program. Usually, the logic of the programs is difficult to be followed by other modellers. The strategy of the SCA is as follows (Sorooshian and Gupta, 1995):

- (1) *Select $p \geq 1$ and $m \geq n+1$, where p = number of complexes, m = number of points in each complex, and n = dimension of the problem. Compute the sample size, $s = p \times m$.*
- (2) *Generate sample S points in the feasible space of parameters. Compute the objective function value at each point. In the absence of prior information, Sorooshian suggests using uniform distributions.*

- (3) *Rank points in order of increasing objective function value.* This rank of points is then stored in an array, D.
- (4) *Evolve each complex according to the Competitive Complex Evolution (CCE) algorithm outlined separately.* The CCE algorithm required for the evolution of each complex in the step (4) of the Shuffled Complex Evolution method (Sorooshian and Gupta, 1995).
- (5) *Shuffle complexes.* Shuffle the complexes by replacing them into D and then sort D in order of increasing objective function value.
- (6) *Check convergence.* This is the step of terminating the process. The process can be stopped after the convergence of errors evaluations is achieved. It means that the algorithms cannot significantly improve the value of the objective function. This condition is considered to indicate arrival at the location of an optimum (please refer to "Function Convergence" and "Parameter Convergence", Sorooshian and Gupta, 1995).

All methods discussed earlier are iterative procedures. Some of them need personal decisions. Therefore, results obtained tend to be different among modellers. Those methods also require high-speed computers. Usually, modellers cannot recognise that the best optimum has already been achieved. Therefore, a function convergence and a parameter convergence are needed to identify the termination.

Theoretically, the advantages of the methods (Sorooshian and Gupta, 1995) are:

- (1) Random numbers can be easily generated and used in the error term of the model.
- (2) Iteration can be repeated many times.
- (3) Subjective factors can be reduced.

Javaheri (1998) reported that the strategy was very successful to calibrate parameters of a Storm Watershed Management Model applied to the Upper Bukit Timah catchment in Singapore. It is indicated by the Nash Coefficient, R^2 values for all storms were close to 1.0.

The typical difficulties of the methods (Sorooshian and Gupta, 1995) are:

- (1) The methods involve very complicated mathematical functions, especially for the non-linear structural characteristics typical of hydrology models.
- (2) The methods are still not able to explain the effects of parameters and interactions.
- (3) Modellers have to develop their own programs, which are very difficult to modify or understand by others.

In view of the inherent weaknesses of the trial and error and numerical optimisation methods for model calibration, the Response

Surface Methodology is proposed to overcome the weaknesses of the previous methods.

Numerical methods will not be used for results' comparison in this study. The reasons are:

- (1) Modellers have to write their own computer programs to apply the methods to their particular model because software of the methods is not available yet.
- (2) Writing the program takes a great deal of time, especially for those who are untrained in computer programming.
- (3) It is usually difficult to follow the logic of the programs written by others, if such a program exist.

2.3. Response Surface Methodology (RSM)

According to Myers and Montgomery (1995) RSM was first introduced by Box and Wilson (1951) based on the theory of "Experiment and Optimum Design" and then further developed by Box and Hunter (1957). Bradley (1958), Davies (1960), and Hunter (1958, 1959a, 1959b) made wide use of the method and developed the strategy of the approach. In hydrology, Liong and Ibrahim (1991 and 1993); and Liong, et. al. (1994) have applied the procedures of Response Surface Methodology to calibrate the Storm Water Management Model (SWMM) parameters for modelling the peak storm runoffs of the Bukit Timah Catchment in Singapore.

The RSM integrates mathematical and statistical techniques, (Myers, R. H. and Montgomery, D. C., 1995. Montgomery, 1997) and was essentially developed from numerical methods. The mathematical techniques are to compute objective functions, to build polynomial models and to optimise the model-parameters. The statistical techniques are to analyse the significance of acceptable results.

The RSM is initiated with an experimental design commonly called design of experiment (DOE) to screen model-parameters before going to the optimisation process (Myers and Montgomery, 1995). The types of the experimental design can be either Factorial or Fractional Factorial Designs (see Chapter 3 for details). The DOE can effectively select the parameters of importance and indicate their interactions that significantly affect the response variables. Therefore, using the DOE, RSM easily optimise the values of model-parameters that are used in the model to produce the best fit between simulated and observed responses.

The benefits of the method (Myers and Montgomery, 1995. Montgomery, 1997. Cornell, 1990) are:

- (1) It can determine the effects of parameter-interactions on the response.
- (2) It has a high ability to guide researchers to select the best model (first, second, or third order polynomials) of response surface to adjust the best value of parameters.
- (3) It is more systematic and accurate in guiding researchers to find the optimum.

- (4) The design and analysis can be conducted using standard statistical software without the need to write custom programs for a particular model.

As a method for model calibration, the procedure is in two stages: Screening Analysis and Optimisation Analysis (Myers and Montgomery, 1995).

Screening analysis using DOE

In general, the purposes of the screening using DOE are to conduct experiments, to select the model-parameters, and to set the range of the model-parameters. In addition, DOE can estimate the effects of parameters and interactions. In this step, modellers have to determine whether a screening experiment is required. If so, an experiment design is created and executed that allows modellers to select the model or process parameters to find the minimum required number of critical experiments. Identification of the critical experiments allows modellers to use response surface methods for the optimisation. DOE that will be used in this research are Factorial Designs and Fractional Factorial Designs. These designs will be discussed later in the Chapter 3.

Analysis using response surface optimisation methods.

In this step, modellers have to create and execute a response surface design. Once the technique analyses the results of the experiment design,

prediction plots are available. Therefore, modellers can quickly identify the important variables using the prediction plots by comparing relative significance of the various terms in the model and selecting those with the greatest impact. The methods allow modellers to build polynomial models based on the effects of parameters and interactions that are recognised using experimental designs. The polynomial models are used to fit the surface graph of responses and to determine the values of parameters and interactions that can achieve the optimum value of responses. Modellers may optimise a single response or a combination of criteria for multiple responses. Optimisation may be to a minimum, maximum or a target value. For combined responses, a specification range may be entered for each of the included responses. With the DOE, researchers can develop statistically exact predictive response surfaces that allow developing a strategy to find the simultaneous targets. The optimum is achieved while using the minimum number of trials. The two popular designs of RSM are Central Composite and Box-Behnken Designs. These designs will be discussed later in Chapter 4.

The RSM requires certain assumptions to simplify the optimisation (Sorooshian and Dracup, 1980). Based on the research of Liong and Ibrahim (1991 and 1993), and Liong, et al. (1994) assumptions used were:

- (1) All parameters are randomly distributed. The type of distribution is usually uniform.
- (2) There are only two ranges of parameters that are considered, upper and lower limits.

- (3) Experimental Designs and Response Surface Methodology are applied to optimise the parameters.
- (4) The relationship between responses and parameters is expressed as a second-order polynomial model:

$$h(X, \varepsilon) = a_0 + \sum_{i=1}^k a_i X_i + \sum_{i=1}^{k-1} \sum_{j=2}^k a_{ij} X_i X_j + \sum_{i=1}^k b_i X_i^2 + \varepsilon \quad (2.3)$$

where

$h(X, \varepsilon)$ = Response surface objective function,

a_0 , a_i and a_{ij} = Coefficients of polynomial models,

X_i and X_j = Parameters of polynomial models.

- (5) The Optimisation is achieved by solving the difference function expressed as

$$h(X, \varepsilon) - h_m = 0 \quad (2.4)$$

where

$h(X, \varepsilon)$ = Fitted response surface,

h_m = Measured system response.

The application of the research by Liong and Ibrahim (1995) was to demonstrate the use of response surface procedures to calibrate a SWMM that was applied in the Upper Bukit Timah, Singapore. Three calibration storms were used to derive the average optimal set of calibration parameters. They analysed 273 experiments to adjust the eight parameters of the Model. The verification was obtained by simulating three additional storms from the average of three calibration storms. The results showed a very good fit between observed and simulated storm runoffs indicated by a low value of the standard error and a high value of the R^2 . They concluded that the RSM was successfully demonstrated on a catchment in Singapore and the simulation was matched to the measured system response.

The next two chapters will explain in detail the two stages of applying the RSM.

Chapter 3

Experimental Designs

In this chapter, commonly used experimental designs will be described. Full Factorial and Fractional Factorial Designs will be described in subsections 3.2 and 3.3, respectively. The selection of three objective functions, which are considered in the response surface optimisation, will be described in subsection 3.4.

3.1. Introduction to Experimental Design

It is very important to have guidance in conducting research especially for research that involves a large number of parameters. Formal experimental designs are thus widely used as the preliminary step in any research methodology (Myers and Montgomery, 1995). The design procedure, commonly known as Design of Experiments (DOE), if properly conducted provides a predictive knowledge of complex and multi-variable processes with the fewest trials possible (Taguchi, 1987a; Lorenzen and Anderson, 1993). Knowing where to run those critical few trials is the key to the technique of DOE (Jazwinski, 1998). Modellers can simultaneously optimise the process for all of the critical outputs to find the best place to achieve the goals once a predictive model exists. DOE deals with optimising

the research processes and maximise the information collected from the process of experimentation, while minimising the cost. In other words, DOE optimises the number of trials required to achieve the best result and to allow drawing valid conclusions about the process. In short, DOE is a systematic process in which some purposeful changes are made to the input variables of a process or system so that we may observe and identify the reasons for changes in the output response. Experiments, if designed and used properly, are also a very powerful research method that can test hypotheses about cause-effect relationships. The essential part of experiments, or experimental research, is good control of all extraneous interference. By keeping extraneous factors under control, the relationships between dependent and independent variables can be observed by manipulating the levels of independent variables, and some kind of cause-effect inference can be made based on the results. The designs of DOE are very useful methods that have already been applied broadly in many disciplines to improve the performance of any process. The benefits of conducting a proper experimental design according to Myers and Montgomery (1995) are:

- (1) Gives unbiased results: DOE select the region of interest or particular points of experiment. Hence, outliers and the results of bias can be avoided.
- (2) Reduces variability and obtain results closer to target requirements: the target requirements are the results that have very low effects of experimental error (error variance due to the different sources of variation

involved in the analysis). Therefore, the prime consideration in the selection of an appropriate design is to reduce the experimental error.

- (3) Is able to estimate effects of factors and interactions: effects that are considered can be statistically tested using statistical tests of significance via an analysis of variance (ANOVA).
- (4) Reduces experimentation time: by analysing only in the particular region or points of interest, researchers can reduce the time for experimentation. Fewer experiments required will also lead to lower overall costs.

The applications of the techniques of DOE usually follow the following strategies as given by Myers and Montgomery (1995):

- (1) *Select the range of model parameters*: This is a lower and upper limit of the parameters in the model of interest. It is important that physical meaning of the range of each be carefully considered. For example, in the case of a rainfall-runoff model, the ranges chosen cannot cause the model to produce negative runoffs.
- (2) *Select the objective function(s)*. The objective functions are used to evaluate the results of the optimisation. Usually, the functions are goodness-of-fit measures. The more objective functions considered, the more precise the optimisation (Kadarisman, 1993). It is more accurate to choose objective functions that will give unbiased results (Lye, 1996). The

objective functions used in this research will be described later in subsection 3.4.

- (3) *Design the experiment*: How the experiment is arranged and carried out is the next step. Many methods exist but the methods that will be used here are 2^k factorial and fractional factorial designs for screening of important parameters, and the methods of Central Composite and Box-Behnken Designs will be used in the optimisation phase. Many off-the-shelf computer programs can be used to design the experiments: for example, Minitab, DOE-PC, Design Expert, Statistica, and SPSS.
- (4) *Estimate effects of parameters and parameter-Interactions*. It is important to consider the interrelationships among parameters and to decide on their levels so that only the important parameters need be considered. The effects are estimated using a standard analysis of variance (ANOVA).

Factorial Designs

Experimental designs in which every level of every variable is paired with every level of every other variable are called factorial designs, (Johnson, N. L., et. al., 1977). A factorial design is a very general kind of design. This can handle any number of treatments or block variables (called factors such as model parameters) and their interactions, these factors can each have any number of categories (called levels). The factorial design then consists of taking the same number of observations for each combination of factor levels. The common experimental designs are Factorial and Fractional Factorial

Designs. When a modeller is interested in the effects of two or more independent variables, it is usually more efficient to manipulate these variables in one experiment than to run a separate experiment for each variable. Moreover, only in experiments with more than one independent variable is it possible to test for interaction among variables. This technique of designs can investigate all possible combinations of the two levels (low and high) of the parameters, (Winner, 1962). In general, the total number of experiments that are used for the designs to analyse the factors (parameters) is based on the number of model-parameters. It means that the total number of required experiments equals two to the power of the number of parameters. The results of the experiments will be used in parameter effect estimation and model fitting and optimisation. The significance of the effects and the coefficients of polynomial models will be examined using "analysis of variance" (ANOVA). The details of the ANOVA table for the factorial design are discussed later.

Contrast and Effect Estimation:

Contrast is a summation of the responses of treatment combinations or experiments. Taguchi (1987a) defined contrasts as the count of total variation that influences the main effect or interaction effect. The contrasts of those parameters and their interactions can be determined using the sign table given in Appendix C, Tables C. 1 and C. 2, for the full two level factorial design and the one half-fractional factorial design, respectively. The results of

the contrast are used for the calculations of effects and the sum of squares. The calculation of the contrasts can be explained in eq. (3.1) for the contrast of A which is easier to explain using only a full factorial design of 2 factors (or parameters), A and B.

$$\text{Contrast A} = \{- (1) + a - b + ab\} \quad (3.1)$$

where:

Contrast A = Contrast value of parameter A

(1) = Response of the process when all parameters are set to the low limit

a = Response of the process when only parameter A is set to the high limit

b = Response of the process when only parameter B is set to the high limit

ab = Response of the process when parameters A and B are set to the high limit

The effect of a parameter or an interaction indicates the influence of the parameter or the interaction to the process or model. It is necessary to study both the effects of main parameters and their interactions. The main effect of an independent parameter is the effect of the parameter averaging over all levels in the experiment. Two independent parameters interact if the effect of one of the parameters differs depending on the level of the other parameter. In some experiments, researchers might find the effect of one main parameter (A) is very small and negligible when the other parameter (B)

is at a low level. However, the effect of A becomes bigger when B is at a high level. This means that the influence of A depends on the level of B. Therefore, knowledge of the interaction AB is as useful as knowledge of the main effect A. The calculation of effects of those parameters and their interactions are given in eq. (3.2). An example for the calculation of the effect of parameter A is:

$$\text{Effect A} = \frac{\text{Contrast.A}}{n2^{k-1}} \quad (3.2)$$

where:

Effect A= Effect value of parameter A

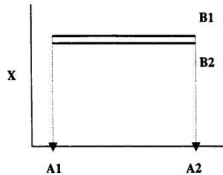
Contrast A= Contrast value of parameter A that calculated using eq. (3.1)

n = Number of replications for each experiment.

k = Number of model parameters.

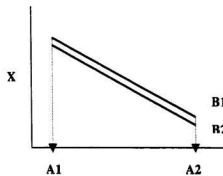
These effects measure the influence of the parameters and interactions to the response. Only parameters that have high effect either positive or negative effect can be considered as variables in the polynomial model. However, to obey the principle of hierarchy, some single parameters sometimes must be included in the polynomial model if some interactions of those parameters are involved in the model, although those single parameters do not have high effect. The visualisation of effects and

interactions can be described using Figures. 3.1.a to 3.1.h. In the diagram, X is the response, A and B are factors.



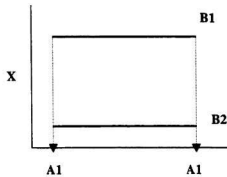
(a)

Fig. 3.1.a Effect Diagram: No effect of factor A, small effect of factor B, and no interaction



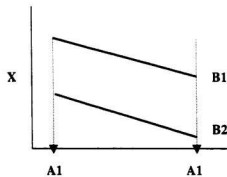
(b)

Fig. 3.1.b Effect Diagram: Large effect of factor A, small effect of factor B, and no interaction



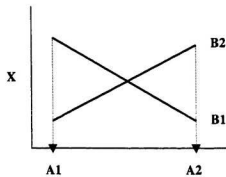
(c)

Fig. 3.1.c Effect Diagram: No effect of factor A, large effect of factor B, and no interaction



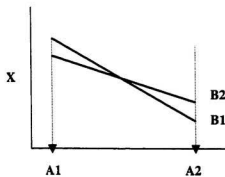
(d)

Fig. 3.1.d Effect Diagram: Large effect of factor A, large effect of factor B, and no interaction



(e)

Fig. 3.1.e Effect Diagram: No effect of factor A, no effect of factor B, and large effect of interaction



(f)

Fig. 3.1.f Effect Diagram: Large effect of factor A, no effect of factor B, and slight effect of interaction

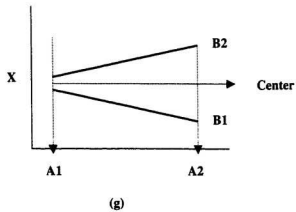


Fig. 3.1.g Effect Diagram: No effect of factor A, large effect of factor B, and large effect of interaction

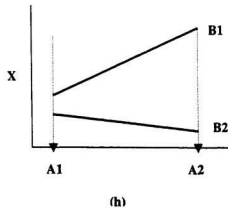


Fig. 3.1.h Effect Diagram: Large effect of factor A, large effect of factor B, and large effect of interaction

Significance of effect of parameters and their interactions can also be evaluated using normal plots of effect and perturbation plots. The normal plot of effect shows the absolute value of the term effects (horizontal axis) against a normal probability scale (vertical axis). Parameters and their interactions that are insignificant will fall on a straight line.

The perturbation plot is useful when trying to decide which axes to use on a contour or 3D plot. The most complex behaviour (most curved or steepest change rate) parameter can be seen in the perturbation plot. The perturbation plot helps modellers compare the effect of all the factors at a particular point in the design space. The response is plotted by changing only one factor over its range while holding all the other factors constant. A steep slope or curvature in a factor shows that the response is sensitive to that factor. A relatively flat line shows insensitivity to change in that particular factor. If there are more than two factors, the perturbation plot should be used to find those factors that most affect the response. The influential factors are good choices for the axes on the contour plots.

The sums of squares of effects defined as the total variation of the individual effect means with respect to the grand mean are calculated from the analysis of variance. Sums of squares of effects are divided by degrees of freedom to produce mean squares. The mean squares of parameter are divided by the mean square of error to produce the significance lack-of-fit test (F_0 -test). The calculation of sums of squares of model parameters and their

interactions can be explained using eq. (3.3). The example for the calculation of the sum of squares of parameter A are calculated using

$$SS_A = \frac{(\text{Contrast}_A)^2}{2^k n} \quad (3.3)$$

where:

SS_A = Sum of squares of parameter A

Contrasts A= Contrast value of parameter A that calculated in eq. (3.1)

k = Number of parameters

n = Number of replications

The sum of squares of error is given by:

$$SS_{\text{error}} = SS_{\text{total}} - \Sigma(SS_{\text{parameters}}) \quad (3.4)$$

where:

SS_{error} = Sum of squares of experimental error

SS_{total} = Sum of squares of the total model

$\Sigma(SS_{\text{parameters}})$ = Summation of all sum of squares of parameter-effects.

The total sum of squares is given by:

$$SS_{\text{total}} = \Sigma(\text{response}^2) - \frac{(\Sigma(\text{response}))^2}{n.2^k} \quad (3.5)$$

where:

SS_{total} = Sum of squares of the total model

$\Sigma(\text{response}^2)$ = Summation of all responses of the experiments

n = Number of replications

k = Number of parameters

The mean of squares can be calculated using:

$$MS = \frac{SS}{df} \quad (3.6)$$

where:

MS = Mean of squares of parameter-effects

SS = Sum of squares of parameter-effects

df = Degree of freedom of parameter-effects

The degree of freedom (df) is an abstract statistical concept in terms of the numbers that are free to vary or the number of independent

components minus the number of parameters. In the case of having only one point, there will be no degree of freedom ($n - 1 = 0$ where $n = 1$) for estimation. In order to plot a regression line, there must be at least two data points. In other words, the degree of freedom tells the number of useful data for estimation. Thus, the lower the degree of freedom, the poorer the estimation. The equations for calculating df of a two-factor experiment are:

$$df_A = (p - 1) \quad (3.7)$$

where:

df_A = Degree of freedom of parameter-effect A

p = Number of possible levels for parameter A

$$df_B = (q - 1) \quad (3.8)$$

where:

df_B = Degree of freedom of parameter-effect B

q = Number of possible levels for parameter B

and

$$df_{AB} = (p - 1) (q - 1) \quad (3.9)$$

where:

df_{AB} = Degree of freedom of interaction-effect AB

p = Number of possible levels for parameter A

q = Number of possible levels for parameter B

The ANOVA allows modellers to test the hypothesis of treatment means using significance tests. The significance test is cast in the form of accepting or rejecting the null hypothesis (H_0), the hypothesis of no difference. If the H_0 is rejected, there will be an alternative hypothesis (H_1). In the ANOVA, the H_0 is accepted or rejected on the basis of the test criterion given by:

$$F_0 = \frac{MS_p}{MS_E} \quad (3.10)$$

where:

F_0 = Value of calculated F- test

MS_p = Mean squares of parameter

MS_E = Mean squares of error

It is common in statistical procedures to use the 5 or 1 percent levels shown in the F table. If the value of F found in the analysis is equal to or greater than the value found in the F table at either the 5 or 1 percent level,

then the H_0 is rejected. In other words, the probability of finding a difference as large as or larger than the obtained value in the experiment is $P \leq 0.05$ or $P \leq 0.01$. Therefore, modellers can conclude that there is a significant difference between the treatment means. The rejecting of H_0 at the 5 percent level means that there is less than 5 percent chance of finding a difference as large as or greater than that of the treatment means. Further detail explanation of ANOVA can be found elsewhere in e.g., Myers and Montgomery (1995).

3.2. Full Two Level Factorial Design

When each factor is applied at two levels, the design is called Two-Level Factorial Design. The term "two levels" means the low level and the high level of the parameters that are considered in the analysis. The levels may be quantitative or qualitative, but in either case are represented by elements of a finite set, usually by $0, 1, 2, \dots, S_i - 1$, where the i -th factor occurs at S_i levels. However, Montgomery (1997) defined that the levels can be set as wide as the real range of the parameter or as close as possible to the predicted value of the known parameter. The creation of full factorial designs with low (-1) and high (+1) levels of each factor means that experiments with two-, three-, or four-factor systems will have four-, eight-, or sixteen-factor combinations or experiments, respectively. In other words, each replicate of the design has exactly 2^k experimental run combinations, in

which k is the number of involved parameters and all parameters have two levels (low and high). Therefore, the design is called 2^k Factorial Designs or Full Factorial Designs (Myers and Montgomery, 1995). The design can be constructed using Yates' forward algorithm or a sign-table. The construction is illustrated below in Tables 3.1 and 3.2, assuming a process with response, Y , that is affected by three factors: A, B, and C.

Table 3.1 Yates' Forward Algorithm Construction Table

| Y | Column 1 | Column 2 | Column3 |
|-----|----------|-------------|------------------------|
| (1) | a+(1) | ab+b+a+(1) | abc+bc+ac+c+ab+b+a+(1) |
| a | ab+b | abc+bc+ac+c | abc-bc+ac-c+ab-b+a-(1) |
| b | ac+c | ab-b+a-(1) | abc+bc-ac-c+ab+b-a-(1) |
| ab | abc+bc | abc-bc+ac-c | abc-bc-ac+c+ab-b-a+(1) |
| c | a-(1) | ab+b-a-(1) | abc+bc+ac+c-ab-b-a-(1) |
| ac | ab-b | abc+bc-ac-c | abc-bc+ac-c-ab+b-a+(1) |
| bc | ac-c | ab-b+a+(1) | abc+bc-ac-c-ab-b+a+(1) |
| abc | abc-bc | abc-bc-ac+c | abc-bc-ac+c-ab+b+a-(1) |

where:

Y = Process that is affected by factors: A, B, and C.

(1) = Response of the process when all factors are set at the low level.

a = Response of the process when only factor A is set at the high level.

b = Response of the process when only factor B is set at the high level.

c = Response of the process when only factor C is set at the high level.

ab = Response of the process when factor a and b are set at the high level.

ac = Response of the process when factor a and c are set at the high level.

bc = Response of the process when factor b and c are set at the high level.

abc = Response of the process when factor a, b, and c are set at the high level.

Column 1 contains of the summation and subtraction of row 1 and 2, 3 and 4, 5 and 6, and 7 and 8 in Column Y.

Column 2 contains of the summation and subtraction of row 1 and 2, 3 and 4, 5 and 6, and 7 and 8 in Column 1.

Column 3 contains of the summation and subtraction of row 1 and 2, 3 and 4, 5 and 6, and 7 and 8 in Column 2.

Therefore:

The effect of factor A = $abc-bc+ac-c+ab-b+a-(1)$ (as shown in Column 3)

The effect of factor B = $abc+bc-ac-c+ab+b-a-(1)$

The effect of interaction AB = $abc-bc-ac+c+ab-b-a+(1)$

The effect of factor C = $abc+bc+ac+c-ab-b-a-(1)$

The effect of interaction AC = $abc-bc+ac-c-ab+b-a+(1)$

The effect of interaction BC = $abc+bc-ac-c-ab-b+a+(1)$

The effect of interaction ABC = $abc-bc-ac+c-ab+b-a-(1)$

Table 3.2 Sign Table

| | A | B | AB | C | AC | BC | ABC |
|-----|---|---|----|---|----|----|-----|
| 1 | - | - | + | - | + | + | - |
| a | + | - | - | - | - | + | + |
| b | - | + | - | - | + | - | + |
| ab | + | + | + | - | - | - | - |
| c | - | - | + | + | - | - | + |
| ac | + | - | - | + | + | - | - |
| bc | - | + | - | + | - | + | - |
| abc | + | + | + | + | + | + | + |

where:

(-) = Sign of factor that is set at the low level.

(+) = Sign of factor that is set at the high level.

The fulfilment of main factor's signs depends on the factor's effect of interest, for example: the fulfilment signs under A, every time a appears will be signed (+), otherwise (-).

The fulfilment of interaction's signs follows the rules of multiplication, for example: $AB = A \times B$, $AC = A \times C$, and $ABC = A \times B \times C$.

Therefore:

The effect of factor A = $abc-bc+ac-c+ab-b+a-(1)$

The effect of factor B = $abc+bc-ac-c+ab+b-a-(1)$

The effect of interaction AB = $abc-bc-ac+c+ab-b+a+(1)$

The effect of factor C = $abc+bc+ac+c-ab-b-a-(1)$

The effect of interaction AC = $abc-bc+ac-c-ab+b-a+(1)$

The effect of interaction BC = $abc+bc-ac-c-ab-b+a+(1)$

The effect of interaction ABC = $abc-bc-ac+c-ab+b-a-(1)$

The results of Yates' forward algorithm are the same as that of the sign table. Applying the design that involves six parameters, the design will suggest 64 experiments to be conducted. The construction of 64 experiments, the total possible combinations from low and high levels of the parameters are shown in Appendix C Table 1.

As the number of parameters increases, the number of runs will also increase rapidly because the number of parameters indicates the value of the

exponent. Modellers have tried to solve this problem using fractional factorial designs, which can reduce the number of runs without neglecting the effect of all parameters and their interactions. Fractional factorial designs will be discussed next.

3.3. Fractional Two-Level Factorial Designs

The fractional factorial designs are invented to attempt to reduce the number of experiments without neglecting the all-main factor effects (Petersen, R. G., 1985). The designs work based on the assumption that alias-parameters (aliases) that appear in the experiments can be neglected. Myers and Montgomery (1995) suggested the alias parameters were recognised using design-generators. The meaning of aliases can be explained as when the effect of one parameter is equal to the other parameters or interactions, then the parameter is called aliased with the other parameters or interactions. For example: Effect $A = \frac{1}{2} (a - b - c + abc)$ and Effect $BC = \frac{1}{2} (a - b - c + abc)$, then, A and BC are aliased (Myers and Montgomery, 1995). Only by neglecting the aliases can the number of experiments be reduced. The types of Fractional Factorial Designs, e. g., One-Half Fractional (OHF) and One-Quarter Fractional (QQF) Designs (Myers and Montgomery, 1995) will be discussed in this chapter. In terms of orthogonality, fractional factorial designs are normally constructed to have both orthogonality and balance; however, they may have more rows than are

required for estimating parameters and error. In such cases, appropriate rows may be trimmed so that orthogonality is preserved but balance is lost.

OHF Designs reduce the number of experiments to a half of the original experiments produced by Two Level Factorial Designs and OQF Designs reduce to a quarter of the original experiments. The number of the experiments for a OHF and OQF are given by:

OHF Designs

$$n = 2^{k-1} \quad (3.16)$$

where:

n = Number of experiments

k = Number of parameters

OQF Designs

$$n = 2^{k-2} \quad (3.17)$$

where:

n = Number of experiments

k = Number of parameters

In the fractional factorial designs, it is important to recognise aliases because recognising aliases will complete the other effects that are not computed in the fractional factorial designs. John (1971) suggested recognising the aliases using the techniques of resolution designs. The technique multiplies design-generators to the main effects to determine the aliases. The design-generator (I) is an interaction factor that contains two, three, or more factors depending on the type of resolution designs and the number of parameters. There are many types of design resolutions (John, 1971); they are named based on the number of factors that are considered to interact into the design-generator. The resolution III design refers to the design that uses three-factor interaction as the design-generator. In addition, the resolutions IV and V indicate the designs that formed using four and five-factor interaction, respectively. There are no resolution I or II designs because the simplest design of factorial is 2^2 (four experiments) and the simplest design does not need any reduction. Consequently, the fractional factorial design is about the reduction of three and more factors (Winer, 1962; John, 1971; and Ogawa, 1974). Moreover, the types of design resolution can be more than five depending on the number of parameters such as the resolution VII design presented by John (1971). However, the solutions will be very complicated and difficult when the number of parameters are very large, such as ten or more. Hydrological modellers usually consider very carefully limiting the number of parameters of a process. The characteristics of resolution III, IV, V, and VI are:

- (1) **Resolution III Designs.** There is no main effect aliased with any other main effect. Main effects are aliased with two-factor interaction. Some other two-factor interactions may be aliased with each other. The design-generator is e. g., $I = ABC$.
- (2) **Resolution IV Designs.** There is no main effect aliased with any other main effect or with any two-factor interaction. However, two-factor interactions are aliased with each other. The design-generator is e. g., $I = ABCD$.
- (3) **Resolution V Designs.** There is no main effect aliased with any other main effect or with two-factor interaction. However, two-factor interactions are aliased with three-factor interactions. The design-generator is e. g., $I = ABCDE$.
- (4) **Resolution VI Design.** There is no main effect aliased with any other main effect, two-, three- or four-factor interaction. However, two-factor interactions are aliased with four-factor interactions. Moreover, three-factor interactions are aliased with each other. The design-generator is e. g., $I = ABCDEF$. More resolutions' characteristics can be determined using the techniques of identification of aliases.

In general, only Resolution V and higher designs are useful. Lower resolution designs would mean that two factor interaction are aliased with other two factor interactions.

3.4. Selection of Objective Functions

Each response in an experiment discussed above indicates the result of the process when the process-parameters are set in a certain arrangement. In this research, the responses are measures of goodness-of-fit between the observation and the Mock-model simulated runoffs. Sorooshian and Gupta (1995) defined that an objective function is an equation that is used to compute a numerical measurement of the difference between the model-simulated output (usually the streamflow hydrograph) and the observed (measured) runoffs. This research considers three objective-functions. The three objective functions are:

- (1) Absolute Sum of Error, $\sum|E|$,
- (2) Nash Sutcliffe Coefficient, R^2 ,
- (3) Deviation of the Runoff Volume, D_v .

Each of the above functions are described below:

a. Absolute Residuals, $\sum|E|$

It is a measure of the absolute differences of the simulated and observed runoffs. The equation of the absolute residuals is expressed as:

$$\sum|E| = \sum_{i=1}^n |Q_s - Q_o| \quad (3.13)$$

where:

$\sum|E|$ = Sum of the absolute residuals

Q_s = Simulated monthly river flows

Q_o = Observed monthly river flows

$\sum|E|$ measures the total experimental errors that occur in the simulation. The units of this measure are equal to the units of the data. Therefore, modellers can directly recognise the differences between simulated and observed data in terms of units. The smaller the value of the measure the better is the fit. A perfect match is when the value of $\sum|E|$ equals zero. Narula (1998) reported that the minimum sum of absolute errors regression is more robust than the least squares regression for some types of outliers because it sums the difference between every single simulated and observed point. Further, it has been proven that even if the value of a certain variable for an observation is changed within limits, it leaves the fitted minimum sum of absolute errors regression unchanged. However, it cannot be used to compare two sets of data that have different number of members, such as different long periods, because the smaller members of data points will automatically produce the smaller amount of $\sum|E|$. Therefore, other objective functions such as R^2 and D_v need to be considered.

b. The Nash Sutcliffe Coefficient, R^2

This measure was invented by Nash and Sutcliffe (1972). The equation of the Nash Sutcliffe Coefficient is expressed as:

$$R^2 = 1 - \frac{\sum_{i=1}^n (Q_o - Q_s)^2}{\sum_{i=1}^n (Q_o - \overline{Q_o})^2} \quad (3.14)$$

where:

R^2 = The Nash-Sutcliffe coefficient

Q_o = The observed monthly river flows

Q_s = The simulated monthly river flows

$\overline{Q_o}$ = The mean of the observed monthly river flows

R^2 measures the experimental errors of simulated values to the grand mean of observed values. The value R^2 is a fraction between 0.0 and 1.0, and has no units. Therefore, R^2 is always less than one. When R^2 equals 0.0, there is no linear relationship between Q_o and Q_s . The measure is akin to the coefficient of determination used in regression analysis. Moreover, it emphasises the ratio of the difference between observed and simulated data to the average of observed data. Therefore, a value of R^2 equals 1.0, does not imply a perfect match, it is only more robust than the absolute residuals to indicate a perfect linear association.

c. The Deviation of the Runoff Volume, D_v

This measurement was given by World Meteorological Organisation (1986) as:

$$D_v = \frac{\sum_{i=1}^n |V_o - V_s|}{\sum_{i=1}^n V_o} \quad (3.16)$$

where:

D_v = The Deviation of the Runoff Volume

V_o = The observed runoff volume

V_s = The simulated runoff volume

D_v measures the percentage of the total experimental errors to the total observed values. Although, D_v equals zero does not indicate a perfect match but more likely measuring the quantity of runoff volume. A smaller value of the measure indicates that the observed and simulated runoff volumes are similar in magnitude.

Chapter 4

Response Surface Methodology (RSM)

In this chapter, the procedure of optimisation using RSM will be presented for calibrating a rainfall-runoff model. Central Composite (CCD) and Box-Behnken (BBD) designs will be described in subsections 4.2 and 4.3 respectively, and followed by subsection 4.4, which explains the use of least squares method for building polynomial models. Analysis of the polynomial models will be presented in subsection 4.5. The last subsection will describe the verification tests on the performance of the calibrated model on selected periods of rainfall data that were not used for the calibration.

4.1. Introduction to Response Surface Methods

The RSM is a method for optimising processes based on polynomial surface analysis (Myers, R. H. and Montgomery, D. C., 1995). Montgomery (1997) notes that Response Surface Methodology (RSM) is a collection of mathematical and statistical techniques that are useful for the modelling and analysis of problems in which a response of interest is influenced by several

variables. Its objective is to optimise the response. Response means the measures of quality characteristics of a system. Here, responses are inputs taken from the results of three objective-functions' computations from selected experiments by the DOE, where, the system concerned here is the Rainfall-Runoff Model. An optimum response is obtained by optimising the polynomial model that is built using the method of least squares. The polynomial model can be easily optimised if there is not any serious multicollinearity that affect the model and if the region of optimum is inside the range of parameters. Multicollinearity problems arise when the predictor variables are highly interrelated, i.e., some predictors or parameters are nearly linear combinations of others. Highly collinear models tend to have unstable regression coefficient estimates. Therefore, to see whether the polynomial can be optimised using trivial solutions, the values of variance inflated¹⁸¹ factor (VIF) or eigenvalues of the polynomial model must be analysed before the optimisation. The VIF measures how much the variance of that model coefficient is inflated by the lack of orthogonality in the design. VIFs exceeding 10 indicate the associated regression coefficients are poorly estimated due to multicollinearity (Cornell, 1990). Eigenvalues, the roots of the polynomial model are required for recognising the physical shape of polynomial models and predicting the location of the global optimum of polynomial model (Burden and Faires, 1989). Another way to see the region of optimum is by plotting 3D graphs called the surface graphs. However, 3D graphs can only be drawn with 2 factors. Therefore, the perturbation plot

should be used to find those 2 factors that most affect the response. The RSM is used to approximate system behaviour, which is highly complex, with a smooth explicit differentiable function (Myers and Montgomery, 1995). The experimental error is defined as variability in the observed values of a product formed from the same set of experimental conditions. The variability is caused by factors that have not been described in the experiment. Therefore, the actual observed values denoted by Y can be expressed (Cornell, 1990) as

$$Y = \eta + \varepsilon \quad (4.1)$$

where:

Y = Actual observed true values

η = Hypothetical observed true values

ε = Experimental errors

The hypothetical simulated values that depend on many levels of factors are denoted by (Cornell, 1990)

$$\eta = \phi (X_1', X_2', X_3', X_4', X_5', \dots, X_k') \quad (4.2)$$

where:

η = Hypothetical true values

X_k' = Levels of factors

The structure of η is usually unknown. Mathematical equations or models called polynomial models that represent main effects, interactions, and intercepts can easily approximate the relationship between η and the levels of factors. The models can be used to fit any kind of phenomenon (Jazwinski, 1998). These models can describe the main effects, curvature effects, and interaction effects. The fitted models can then be used to draw pseudo-three-dimensional response surface plots. First-order polynomial models, the simplest forms, can only explain plane surface regions while higher-order models such as second-order or third-order polynomial models can fit curved surfaces. However, the third order polynomial models that are developed by response surface are mostly aliased with the second order (Cornell, 1990). Therefore, it is not used here. The first-order and second-order polynomial models (Myers and Montgomery, 1995) are expressed as eq. (4.3) and (4.4), respectively.

$$y = \beta_0 + \sum_{i=1}^k \beta_i x_i + \sum_{i < j} \beta_{ij} x_i x_j \quad (4.3)$$

$$y = \beta_0 + \sum_{i=1}^k \beta_i x_i + \sum \beta_{ii} x_i^2 + \sum_{i < j} \beta_{ij} x_i x_j \quad (4.4)$$

where:

y = Response

β = Coefficients

x = Parameters

k = Number of parameters

Parameters and interactions of parameters that are considered involved in the polynomial model are selected based on the effect estimation and the principle of hierarchy. After having the form of the polynomial model, then the estimates intercept (β_0), main effects (β_1, β_2, \dots), curvature effects ($\beta_{11}, \beta_{22}, \dots$), and interaction effects ($\beta_{12}, \beta_{23}, \dots$) are derived using the method of least squares to complete the polynomial model.

In RSM, contour plots, which results from the polynomial model can help in visualising the shape of the three-dimensional response surface (Cornell, 1990). The contour plots are drawn on a graph whose coordinates represent the levels of the factors. The use of the contour is to indicate the different surface height values, which leads modellers to focus on the specific experimental region of interest. The experimental region of interest is the region of conceivable factor level values that represents the factor combination of potential interest.

The region can also be determined by specifying the value of each factor that represents the current operating conditions. Applications of the RSM technique include (Liong and Ibrahim, 1991):

- (1) Approximating the behaviour of tubular joint of an offshore structure;
- (2) Estimating the reliability of primary-secondary system;
- (3) Approximating the behaviour of structure subjected to earthquake loads;
- (4) Studying the effects of uncertainties on dynamic response of soil-structure interaction;
- (5) Estimating fatigue reliability of components.

There are many design types of Response Surface Methodology: Central Composite, Box-Behnken, Three-Level Factorial, Hybrid, D-Optimal, Distance-Based, Modified-Distance designs, etc. (Myers, et al, 1995; and Cornell, 1990). The Central Composite Design is the most frequently used because it is less complicated. The Box-Behnken Design is also recommended by many experts (Myers and Montgomery, 1995) because it needs the least number of required experiments under certain conditions. Therefore, only Central Composite Designs (CCD) and Box-Behnken (BBD) designs will be used in this thesis. These are described in Subsections 4.2 and 4.3, respectively.

The Central Composite Design (CCD) introduced by Box and Wilson in 1951 is the most popular design to fit second-order designs (Myers and Montgomery, 1995). The design is created from either factorial or fractional factorial designs. The design can flexibly focus the region of interest based on the axial distances and the number of centre runs. This design will be applied in this research, and will be described later.

The Box-Behnken Design (BBD) was developed by Box and Behnken in 1960. The design is an efficient method of fitting a second-order polynomial model for the optimisation designs (Myers and Montgomery, 1995). The design needs fewer experiments than other designs because it is created from either fractional factorial or a balanced incomplete box (John, 1971; Sorooshian and Arfi, 1982; and Myers and Montgomery, 1995). The design will be applied in the research. Therefore, it will be described later.

Activities that must be carried out to use the RSM are:

- (1) Select the appropriate design (RSM-design). The types of RSM-designs have already been discussed above. Details for CCD and BBD will be described later.
- (2) Conduct the experiments based on the type of DOE arrangement. The type of DOE has already been discussed in Chapter 3.
- (3) Calculate objective functions for each experiment as responses. The objective functions have already been discussed in Chapter 3.
- (4) Establish polynomial models. The polynomial models can be established using the method of least squares.
- (5) Analyse the polynomial model using ANOVA to test for goodness-of-fit of the polynomial model, and perform residual plots, contour and surface plots, and perturbation plots. The plots, which are discussed later, are used to identify outliers. The contour and surface plots, which are discussed later, are used to help identify the optimum response.
- (6) Obtain the variables of the polynomial model by estimating the coordinates of the stationary point of the second-order polynomial model using partial derivative methods.

The iterative DOE-RSM procedures are shown in Fig. 4.1

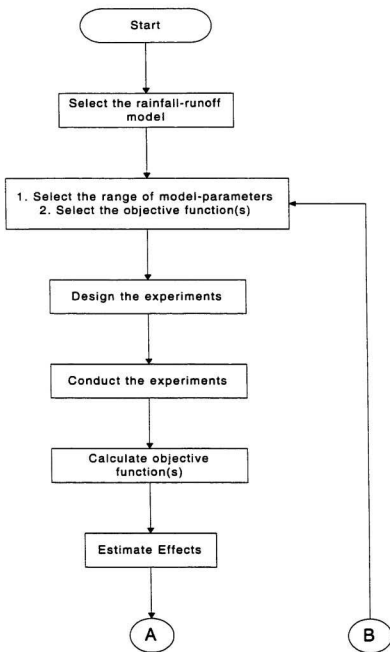


Fig.4.1.a. DOE Iterative Procedure

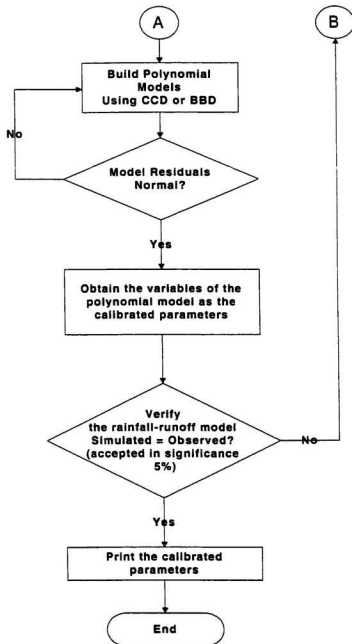


Fig.4.1.b. RSM Optimisation Iterative Procedure

4.2. Central Composite Designs (CCD)

Central Composite Designs are used to investigate the simultaneous effects of two or three continuous variables on the performance characteristics of products and processes in research, development, and manufacturing. Central Composite Designs (CCD) are formed originally from the two level factorial designs augmented by additional points to allow the coefficients of a second-order model to be estimated (Unal, 1994 and Montgomery, 1991). The additional points are axial points and centre points as shown in Fig. 4.2.

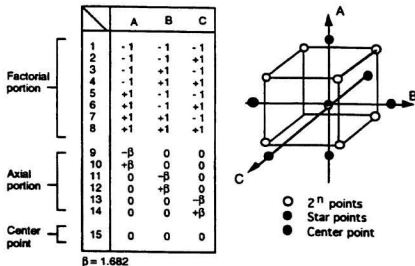


Fig.4.2 Experimental design for three factors: A, B, and C

In other words, the centre points are used for the evidence of curvature investigation (Myers and Montgomery, 1995). The curvature is identified using the significance F-test of curvature analysed using sum of squares and mean of squares of curvature. The equation for the sum of squares of curvature (Myers and Montgomery, 1995) is expressed as

$$SS_C = \frac{n_F n_C (\bar{y}_F - \bar{y}_C)^2}{n_F + n_C} \quad (4.12)$$

where:

SS_C = Sum of Square of Curvature;

n_F = Number of factorial design points;

n_C = Number of additional replicates of central point;

\bar{y}_F = Average observations of factorial designs;

\bar{y}_C = Average runs at the central point.

The equation for the mean of squares of curvature (Myers and Montgomery, 1995) is expressed as

$$MS_C = SS_C / df_C \quad (4.13)$$

where:

MS_C = Mean of squares of curvature;

SS_c = Sum of squares of curvature;

df_c = Degrees of freedom of curvature.

The equation for the mean of squares of error affected by curvature (Myers and Montgomery, 1995) is expressed as

$$MS_e = SS_e / (n_c - 1) \quad (4.14)$$

where:

MS_e = Mean of squares of error;

SS_e = Sum of squares of error (it has been discussed in Chapter 3);

n_c = Number of centre points.

The equation for the F-ratio of curvature (Myers and Montgomery, 1995) is expressed as

$$F\text{-ratio}_c = MS_c / MS_e \quad (4.15)$$

where:

$F\text{-ratio}_c$ = Calculated F-ratio of curvature;

MS_c = Mean of squares of curvature;

MS_e = Mean of squares of error.

The evidence of curvature can be investigated by comparing the value of calculated F-ratio to F-ratio on the table. Therefore, polynomial models that are established using CCD are more accurate than those of two-factorial design, because CCD applies centre points (Myers and Montgomery, 1995). Central Composite designs are orthogonal in that all the parameters for the CC model may be estimated, but the design itself is unbalanced. A greater or lesser number of centre points is used to achieve an estimating criterion and an error estimate (Cornell, 1990).

A CCD can be made rotatable. Rotatability is a desirable property relating to the precision of the predicted response value. An experimental design is rotatable if the variance of the estimated response depends on the distance from the design centre and not on the direction (Cornell, 1990; Unal, 1994; and Myers and Montgomery, 1995). In other words, rotatability ensures that the error in prediction stays constant around the design (Barker, 1985). For achieving the rotatable condition, the distance of axial points is determined using the equation (Myers and Montgomery, 1995)

$$\alpha = \sqrt[k]{F} \quad (4.16)$$

where:

α = Axial distance;

F = Number of factorial points = 2^k ;

k = Number of parameters.

The condition of rotatability for the designs of six parameters can be achieved using the axial distance of $\alpha = 2.828$. The experiments on this research based on Central Composite Design are shown in Appendix B Table 28. After having the additional points including the axial points, then the required number of experiments based on Central Composite designs can be expressed using the eq. (4.10) below (Myers and Montgomery, 1995)

$$n = 2^k + C \quad (4.17)$$

where:

n = Required number of experiments;

k = Number of parameters;

C = The Number of additional points.

4.3. Box-Behnken Designs (BBD)

In the case of the designs having a large number of experiments, Box and Behnken (1960) have developed highly fractionalised designs to screen the maximum number of (main) effects in the least number of experimental experiments. These designs are constructed by combining two-level factorial designs with incomplete block designs, and have complex confounding of interaction (Box and Draper, 1969). The analysis of these types of designs proceeds in the same way as was described in the context of fractional

factorial designs. However, for each effect, modellers can now test for the linear effect and the quadratic (non-linear effect). For example, when studying the yield of a chemical process, temperature may be related in a non-linear fashion, that is, the maximum yield may be attained when the temperature is set at the medium level. Thus, non-linearity often occurs when a process performs near its optimum. Technically, Box-Behnken designs can also be constructed by fractionalising a full three-level factorial design so that only the centre point and the edge points of the hyper-cube are used. These designs are alternatively formed by combining two-level factorial designs with incomplete block designs (Unal, 1994). Box-Behnken designs are used to acquire data for a full second-order-polynomial model that will describe in detail the system or process being investigated. The construction of Box-Behnken Designs can be explained as in Table 4.1.

Table 4.1 The Box-Behnken Constructing Table

| | Treatment | | |
|-------|-----------|----|----|
| | A | B | C |
| exp_1 | H* | H* | L* |
| exp_2 | H* | L* | H* |
| exp_3 | L* | H* | H* |
| exp_4 | H* | H* | C* |
| exp_5 | H* | C* | H* |
| exp_6 | C* | H* | H* |
| exp_7 | C* | C* | C* |

where

A, B, and C = Parameters;

exp_1, 2, ... = Experiments number 1, number 2, ...;

H* = The Highest value of parameter;

L* = The Lowest value of parameter;

C* = The central value of parameter.

Therefore, the required number of experiments based on Box-Behnken designs can be expressed using the eq. (4.4) below:

$$n = 2^M + C^* \quad (4.18.a)$$

$$M = (k-1) \quad (4.18.b)$$

where

n = Required number of experiments;

k = is the number of parameters;

C* = The number of central points.

The designed experiments based on the Box-Behnken Design for this research are shown in Appendix B Table B.2.

4.4. Least Squares Method For Establishing Polynomial Models

The simple and common method to obtain parameter estimates is the least squares method (Beck and Arnold, 1976). Beck and Arnold recommended using the method, particularly when nothing is known regarding the measurement errors. Myers and Montgomery (1995) defined that the principle of least squares asserts that a set of estimates of parameters can be obtained by minimising the sum of experimental errors ($\sum \varepsilon$). This principle of estimation can be used to establish the polynomial models commonly known as the technique of regression using least squares estimation. There are many references containing the process of building the polynomial model. It, therefore, is not explained in this thesis. However, it can be found in, e. g., Myers and Montgomery (1995), Devore (1995).

The polynomial model establishments must obey the principle of hierarchy. Cornell (1990) defines hierarchy as the ancestral lineage of effects flowing from main effects (parents) down through successive generations of higher order interactions (children). For statistical reasons, models that contain subsets of all possible effects should preserve hierarchy. Although the response may be predicted without the main effects when using the coded variables, predictions will not be the same in the actual variable levels unless the main effects are included in the model. Without the main effects, the model will be scale-dependent.

4.5. Polynomial Model Analysis

The polynomial models that are established must be analysed using ANOVA to obtain the best model to fit the response surface. These analyses include determining:

- (1) The level-order of polynomial model;
- (2) The coefficient of every factor or parameter;
- (3) The validity of the assumptions of the model.

The level order of the polynomial model is tested using the sum of squares of curvature that is expressed as the eq. (4.12); the coefficient of every factor is analysed using the eq. (4.13), (4.14), and (4.15). The residuals, which are obtained from the difference between, observed values and predicted values of responses must also be analysed to check the validity of all the statistical tests. The residuals should be independent, homoscedastic, and normally distributed. The residuals must also be checked for outliers and that no observation is unduly influencing the results. All these tests are standard tests normally carried out in a regression analysis and hence will not be discussed further here.

4.6.Verification Procedures

The accuracy of calibration must of course be proved using a verification scheme. This is because the results of any calibration process are conditional on several factors, for example: the calibration data, the objective function, and the optimisation procedure. For verification, the calibrated parameters must be used in the model to simulate runoffs beyond the years of the calibration periods. Then, the simulated runoffs are compared with the observed runoffs of the same years. This verification will use a two-year rainfall period, 1977 to 1978 to simulate two-year runoffs by using the parameters from the calibration in the Mock Model using four scenarios. This is illustrated in Fig. 4.3.

| | | | | | |
|-------------|---|---|---|--------------|------|
| 1973 | - | - | - | 1977 | 1978 |
| Calibration | - | - | - | Verification | |

Fig. 4.3.a Calibration Using One-Year Data to Estimate Two-Year Runoffs In Verification

| | | | | | |
|-------------|------|---|---|--------------|------|
| 1973 | 1974 | - | - | 1977 | 1978 |
| Calibration | | - | - | Verification | |

Fig. 4.3.b Calibration of Two-Year Data to Estimate Two-Year Runoffs In Verification

| | | | | | |
|-------------|------|------|---|--------------|------|
| 1973 | 1974 | 1975 | - | 1977 | 1978 |
| Calibration | | | - | Verification | |

Fig. 4.3.c Calibration of Three-Year Data to Estimate Two-Year Runoffs In Verification

| | | | | | |
|-------------|------|------|------|--------------|------|
| 1973 | 1974 | 1975 | 1976 | 1977 | 1978 |
| Calibration | | | | Verification | |

Fig. 4.3.d Calibration of Four-Year Data to Estimate Two-Year Runoffs In Verification

The longer period of time for which data is available to calibrate the model will produce the more accurate future prediction. However, in some cases, modellers may have limited data. Therefore, using the four scenarios of verifications above, modellers can estimate the accuracy of each period of calibration to predict the future runoffs.

Chapter 5

Mock Rainfall-Runoff Model

This chapter will describe the Mock Rainfall-Runoff Model in general, which will be used as illustration of the use of RSM for calibrating rainfall-runoff models. The complete description of Mock Rainfall-Runoff Model can be found in Mock (1973).

5.1. Mock Rainfall Runoff Model Description

Runoff is an element of the hydrologic cycle that appears on the earth's surface. Surface runoffs that occur in tropical countries, e.g., Indonesia, are caused by rainfall. In general, the amount of rainfall that causes the runoff is the total amount of effective rainfall in the basin after subtraction of evapotranspiration, infiltration, and other minor losses. Evapotranspiration and infiltration are influenced by three main factors: climate, topography, and soil characteristics. Therefore, rainfall-runoff models developed to simulate the rainfall-runoff process must involve these factors. These models can be classified as either theoretical or empirical models (Wiest, 1965). A theoretical model includes a set of general laws or theoretical principles. If all the governing physical laws were well known and could be described by equations of mathematical physics, the model would

be physically based. An empirical model omits the general laws and is in reality a representation of observed data. Depending on the character of the results obtained, models are classified as stochastic or deterministic. If one or more of the variables in the mathematical model are regarded as random variables having a probability distribution, then the model is stochastic. If all the variables are considered free from random variation, the model is deterministic.

Most existing rainfall-runoff models are physically based deterministic models because catchment characteristics are represented by fixed model parameters (Liong and Ibrahim, 1994). Examples of rainfall-runoff models include: HEC-1 Flood Hydrograph Package (Feldman, 1981), Tank Model (Sugawara, 1974), Xinanjiang Model (Zhao, 1992), University of British Columbia (UBC) Watershed Model (Quick, 1977), Streamflow Synthesis and Reservoir Regulation (SSARR) Model (Rockwood, 1982), Hydrological Simulation Program Fortran (HSPF) (Donigian, 1984), and Mock Rainfall-Runoff Model (Kadarisman, 1993 and Kurniawan, 1994)

The Mock Rainfall-Runoff Model that will be used as illustration in this research was developed in Indonesia to calculate monthly water availability for water management purposes (Mock, 1973). This model is commonly used for irrigation planning. The calculation of resulting runoff uses rainfall and evapotranspiration as inputs, and six soil characteristic factors as the model parameters. The Mock model is quite simple to use because only six parameters (soil impermeable layer, coefficient of infiltration, coefficient of

recession, soil moisture capacity, initial soil moisture, and initial storage value) are involved in the calculation. However, these six parameters must be calibrated for the catchment of interest before its use. In this thesis, the Mock Model will be used to model the monthly water availability on the Babak River Catchment in Lombok, Indonesia. The rainfall data were taken from the Department of Hydro-Meteorology in Indonesia. The rainfall data are presented in Appendix E Table E.1, as well as evapotranspiration and historical runoff data.

5.1.1. Effective Rainfall

Rainfall data (P) is the main input to the runoff process. The rainfall data used in the calculation is the average rainfall data from gauging stations in the basin. This average is approximated using the well-known Thiessen polygon method (Harto, S., 1993; Soemarto. C. D., 1995; and Lye. L. M., 1996).

5.1.2. Evapotranspiration

It is difficult to measure evapotranspiration directly in the field; therefore, in general, it is estimated based on measured climatic data. Mock (1973) suggested using the Penman method (Mock, 1973 and Soeprapto, 1994) because the Penman method uses more variables than other methods.

The evapotranspiration can be obtained either using Penman's equations or interpolating from the tabulated values to determine the amount of monthly evapotranspiration. The calculated evapotranspiration data used herein were taken from the Department of Hydro-Meteorology, Indonesia.

5.1.3. Calculation of water balance

The Mock model calculates the rainfall-runoff of a catchment on a monthly basis. Runoff (RO) of a river is directly affected by the amount of monthly baseflow (bf), direct runoff (dro), and storm-runoff (storm) (Mock, 1973). Each element will be described later. RO is mathematically expressed as

$$RO = bf + dro + storm \quad (5.2)$$

where:

RO = Amount of catchment runoff

bf = Amount of monthly baseflow

dro = Amount of direct runoff

storm = Amount of storm runoff

Mock (1973) explained that monthly baseflow (bf) can be calculated based on the amount of infiltration in the particular month after subtracting the monthly change of storage volume. It is expressed as

$$bf = i t - \Delta V_n \quad (5.3)$$

where:

bf = Monthly baseflow

i t = I = Infiltration in the particular month

ΔV_n = Monthly change of storage volume

Mock (1973) defined the infiltration rate, I, based on the coefficient of infiltration and the availability of water surplus. The equation of the infiltration rate is expressed as:

$$I = COI \times WS \quad (5.4)$$

where:

I = Infiltration rate

COI = Coefficient of infiltration

WS = Water surplus

Mock (1973) defined Water surplus, WS, as the excess of precipitation over evapotranspiration by considering the amount of soil moisture. The water surplus is calculated using the equation below.

$$WS = Pr - Ea \quad (5.5)$$

where:

WS = Water surplus

Pr = Amount of monthly rainfall (precipitation)

Ea = Effective evapotranspiration

Mock (1973) defined Storage volume, V, at the time T calculated based on the coefficient of recession, the previous storage volume, and the infiltration rate. The equation to calculate the storage volume is:

$$V_t = K V_{t-1} + \frac{1}{2} (1 + K) I \quad (5.6)$$

where:

V_t = Storage volume

V_{t-1} = Previous storage volume

K = Coefficient of recession

I = Infiltration rate

Mock (1973) differentiated rainfall-runoffs into two categories, Direct runoff, dro and Stormrunoff, storm. Mock defined dro as the difference between the available water surplus and the infiltration rate. The equation to calculate direct runoff is given by:

$$\text{dro} = \text{WS} - I \quad (5.7)$$

where:

dro = Direct runoff

WS = Water surplus

I = Infiltration rate

Mock (1973) then defined storm runoff as the amount of initial precipitation, which occurs in the beginning of raining season that cannot be infiltrated into the ground. The storm runoff occurs because the outer surface layer is still very dry and the infiltration capability is still very low. This condition is affected by the percentage of impermeable layer and calculated using:

$$\text{storm} = \text{Pr} \times \text{IMLA} \quad (5.8)$$

where;

storm = Amount of storm runoff

Pr = Amount of precipitation (rainfall)

IMLA = Percentage of impermeable layer.

5.2. Parameters of the Mock Model

Mock (1973) defined six parameters in his model: coefficient of Impermeable layer ($imla$), initial storage value (V_o), coefficient of Infiltration (COI), soil moisture capacity (SMC), monthly coefficient of recession (K) and initial soil moisture (SM_o). The range of all parameters must be known before the calibration process. In general it is better to have a smaller range or otherwise, it may be difficult to find the optimum values of the parameters because the wider the range, the flatter will be the response surface.

a. Impermeable Layer, $imla$

Mock (1973) described the range of this parameter between 8 % to 12 % or (0.08 to 0.12). It has a positive effect on the storm runoff. It means that it also has positive effect to the direct runoff and monthly flows.

b. Initial Storage Value, V_o

This parameter is the previous amount of storage value. The storage value has negative effect to the direct runoff. According to Kadarisman (1993), the range of this parameter is between 150 to 250 mm.

c. Coefficient of Infiltration, COI

According to Soeprapto, M., (1994), the COI has a range between 0.35 to 0.65 mm. It has a positive effect to the amount of infiltration. It means that it also has negative effect to the direct runoff and monthly flows.

d. Coefficient of Recession, K

Kadarisman (1993) specified that the range of K is between 0.6 to 0.8. It has a positive effect to the amount of storage volume. It means that the amount of storage volume will increase simultaneously as K increases.

e. Soil Moisture Capacity, SMC

This parameter is for the use of water surplus calculation. It has a negative effect to the amount of direct runoff. Mock (1973) explained that the range of this parameter is between 180 to 220 mm.

f. Initial Soil Moisture, SM_i

This parameter is the previous amount of soil moisture. The summation of this amount to the precipitation will be compared to the amount of soil moisture capacity. The range of this parameter is between 190 to 210 mm.

Although, every model-parameter has a particular range in the real field, modellers have to be very careful to set the range of those model-parameters in calibration processes. A wide range of parameters may lead to unresolved results of calibrations because the optimisation process may be trapped and terminated in an incorrect result, for example: in a local optimum. A wide range can also lead to an error calculation of a particular computer program. Similarly, a narrow range may also lead to an unresolved result because the location of optimum result is beyond the range. Therefore, it is better for modellers to use the guidance of DOE to determine the specific range of those parameters, which are more appropriate for the Calibration of Mock rainfall-runoff model using RSM. Later in Subsection 1, Chapter 6, the parameters' range determination is described following to the description of effect estimations.

The Mock Rainfall-Runoff Model Parameters with the codes for the calibration are presented in Table 5.1 below.

Table 5.1. The mock model parameters

| Parameters | | Code | Units | Low Level | High Level |
|----------------------------|--------|----------|-------|-----------|------------|
| % of Impermeable Layer | IMLA | A | - | 0.08 | 0.12 |
| Initial Storage Value | V_0 | B | mm | 150 | 250 |
| Coef. of Infiltration | COI | C | - | 0.35 | 0.65 |
| Monthly Coef. of Recession | K | D | - | 0.6 | 0.8 |
| Soil Moisture Capacity | SMC | E | mm | 180 | 220 |
| Initial Soil Moisture | SM_0 | F | mm | 190 | 210 |

5.3. Logic of the Mock Model

The logic of the Mock model is presented in the flowcharts shown in Fig. 5.1.a. and Fig. 5.1.b. Different sub-calculations are sometimes necessary in the calculation, depending on the value of the parameters. The different conditional cases for sub-calculation are also shown as a flow chart in Fig. 5.2.

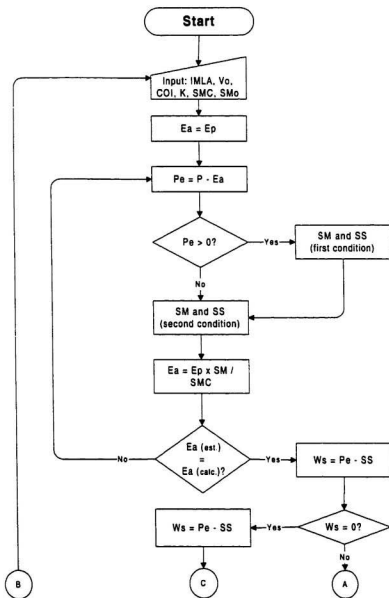


Fig. 5.1.a. The Mock Rainfall-Runoff Model Flow Process (part one)

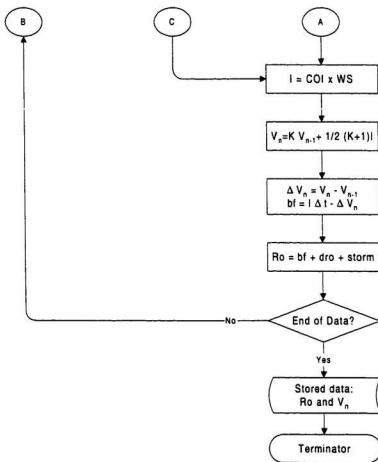


Fig. 5.1.b. The Mock Rainfall-Runoff Model Flow Process(part two)

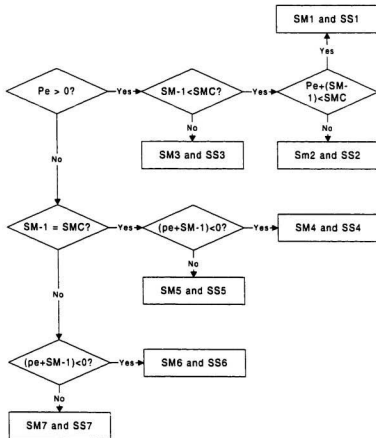


Fig. 5.2 Sub-Calculation Based On Different Conditions

Chapter 6

Results and Discussions

Results of the model calibration and the verification are discussed in this chapter. The results and discussions start systematically from effect estimations, minimum required number of experiments, analysis of polynomial model for optimisation, final calibrated parameters, and the results of model verification.

6.1. Effect Estimations

Effect estimations using Full Factorial (FF) and One-Half Fractional Factorial (OHF) resolution VI are compared and shown in Table 6.1. The effect analyses based on the three responses (sum of absolute residuals $|E|$, R^2 , and Dv) produced similar results. Hence, only the effects based on the response of sum of absolute residuals, $|E|$, are presented as representative of the other responses. The objective was to minimise the sum of the absolute residuals.

The Mock model parameters: IMLA, V_o , COI, K, SMC, and SM0 are represented by the letters A, B, C, D, E, and F, respectively. The table shows all effect estimations except the effects of alias factors. The high effect factors and additional factors will be used to establish the polynomial model for the

optimisation phase. The additional factors are factors that although have relative low effect, must still be included into the polynomial model to obey the principle of hierarchy.

Table 6.1 The Effect Estimation based on the response of absolute residuals calculated using FF and OHF Designs

| Par/Interac. | Effects | |
|--------------|----------|----------|
| | Full | OHF |
| A | 0.978906 | 1.288438 |
| B | 26.17097 | 26.16119 |
| AB | 0.589781 | 0.701437 |
| C | 228.1398 | 228.1407 |
| AC | 0.589781 | 0.701437 |
| BC | -10.7546 | -10.7456 |
| ABC | -2.52078 | -3.34631 |
| D | -83.6533 | -83.6552 |
| AD | 9.903281 | 9.865063 |
| BD | -16.9645 | -16.9744 |
| ABD | 0.828156 | 0.829062 |
| CD | 318.0513 | 318.0526 |
| ACD | 0.828156 | 0.829062 |
| BCD | 0.009559 | =AEF |
| ABCD | -0.69591 | =EF |
| E | 66.30784 | 66.30631 |
| AE | -1.04122 | -0.73169 |
| BE | -27.2814 | -27.2912 |
| ABE | -0.32909 | -0.21744 |
| CE | -13.8896 | -13.8887 |
| ACE | -0.32909 | -0.21744 |
| BCE | 8.697781 | =ADF |
| ABCE | -0.83447 | =DF |
| DE | 22.72134 | 22.71944 |
| ADE | 0.755906 | 0.717687 |
| BDE | 16.60334 | =ACF |
| ABDE | -0.56697 | =CF |
| CDE | -1.05853 | =ABF |
| ACDE | -1.00328 | =BF |
| BCDE | 3.831531 | =AF |
| ABCDE | 0.433219 | =F |

| | | |
|--------|----------|----------|
| F | -3.72828 | -3.29506 |
| AF | 0.009406 | -1.28844 |
| BF | 1.031469 | -26.1612 |
| ABF | 0.001281 | -0.70144 |
| CF | 1.200906 | -1.22101 |
| ACF | - | -15.4227 |
| | 15.45996 | |
| BCF | -0.03822 | =ADE |
| ABCF | -0.00191 | =DE |
| DF | -0.82553 | -0.83655 |
| ADF | 9.03114 | 9.86506 |
| BDF | -0.56403 | =ACE |
| ABDF | 0.000906 | =CE |
| CDF | 0.111656 | =ABE |
| ACDF | 0.000906 | =BE |
| BCDF | 0.309531 | =AE |
| ABCDF | -0.00153 | =E |
| EF | -3.72828 | -3.63063 |
| AEF | 0.009406 | 0.731687 |
| BEF | 1.031469 | =ACD |
| ABEF | 0.001281 | =CD |
| CEF | 1.200906 | =ABD |
| ACEF | 0.001281 | =BD |
| BCEF | -0.03822 | =AD |
| ABCEF | -0.00191 | =D |
| DEF | -0.82553 | =ABC |
| ADEF | 0.009031 | =BC |
| BDEF | -0.56403 | =AC |
| ABDEF | 0.000906 | =C |
| CDEF | 0.111656 | =AB |
| ACDEF | -0.00978 | =B |
| BCDEF | 0.309531 | =A |
| ABCDEF | -0.00153 | =I |

Table 6.1 shows that, FF and OHF generally gave similar results, especially those for high effects. Among the 63 factor effects, the main parameters B, C, D, and E have high effects on the response. The highest and the second highest effect parameters being C (Coefficient of Infiltration) and D (Recession constant), respectively.

For two-parameter interactions, BC, AD, BD, CD, BE, CE, and DE are considered to have high effects. Fig. 6.1 to Fig. 6.14 show the relationship among these interactions. There is no interaction of more than two parameters having a high effect.

Two-factor interactions:

Parameters B and C

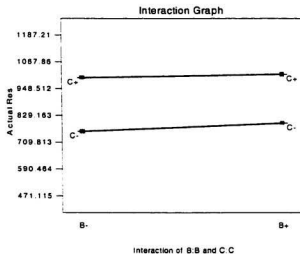


Fig.6.1 Relationship Between Parameters B and C

Parameter B has positive effect on the change of the process as shown in Fig. 6.1. It means that increasing parameter B will increase the yield (response) of the process. However, the interaction of this parameter with parameter C, that has very high positive effect, will have high negative effect

to the change of the process. Figure 6.2, shows the three-dimensional surface graph of parameters B, C and the response.

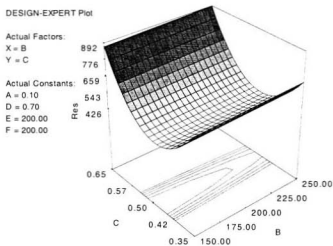


Fig. 6.2 Three-dimensional graph of the relationship among parameters B, C, and the yield of the process (|E|).

As shown in Fig. 6.2, to minimise the response of the process, the value of parameter B is somewhere between 150 and 200, and the value of parameter C is between 0.45 and 0.50.

Parameters A and D

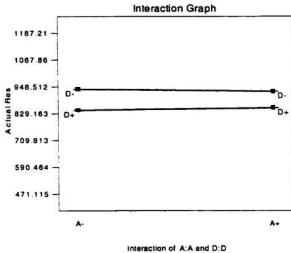


Fig. 6.3 Relationship Between Parameters A and D

Parameter A, as shown in Fig. 6.3, has small positive effect to the change of the process. However, according to the effect estimation, it will have high positive effect while interacting with parameter D that has a high negative effect. From Fig. 6.4, the three-dimensional graph of the relationship among parameters A, D, and the response, shows the region of prediction values of the parameters. Fig. 6.4 shows that the minimum yield of the process will be achieved when the value of parameter A is somewhere between 0.08 and 0.11, and the value of parameter D is somewhere between 0.70 and 0.75. Beyond those values, the yield of the process will not be the minimum.

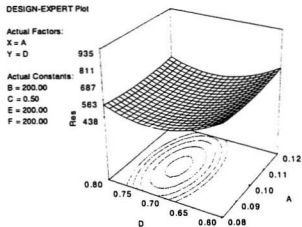


Fig. 6.4 Three-dimensional graph of the relationship among parameters A, D, and the yield of the process.

Parameters B and D

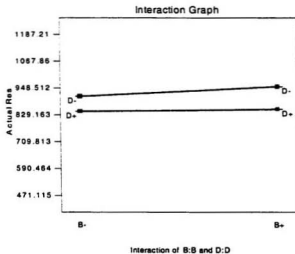


Fig. 6.5 Relationship Between Parameters B and D

The interaction between parameters B and D are shown in Fig. 6.5. In this case, increasing parameter B, while decreasing parameter D will increase the yield of the process. However, as shown in Fig 6.6, the minimum of the process' yield will be achieved when the value of parameter B is somewhere between 150 and 200, and the value of parameter D is between 0.68 and 0.73.

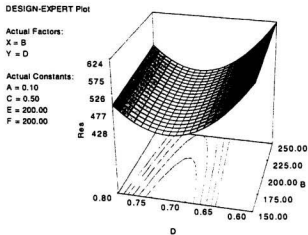


Fig. 6.6 Three-dimensional graph of the relationship among parameters B, D, and the yield of the process

Parameters C and D

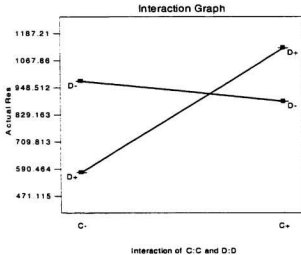


Fig. 6.7 Relationship Between Parameters C and D

Fig. 6.7 shows that the interaction of parameter C, which has a positive effect, on parameter D, which has a negative effect, will increase the yield of the process. It means that the increase of C and the decrease of D will increase the value of response. However, the objective is to set the parameters to minimise the response. Therefore, to reduce the response, parameter C must be decreased and parameter D must be increased. Further as shown in Fig. 6.8, the optimum process' yield is achieved when the value of parameter C is somewhere between 0.45 and 0.55, and the value of parameter D is between 0.72 and 0.78.

DESIGN-EXPERT Plot

Actual Factors:

X = C

Y = D

Actual Constants:

A = 0.10

B = 200.00

E = 200.00

F = 200.00

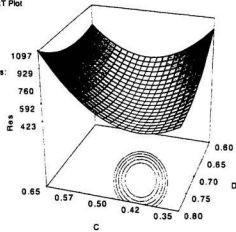


Fig. 6.8 Three-dimensional graph of the relationship among parameters C, D, and the yield of the process

Parameters B and E

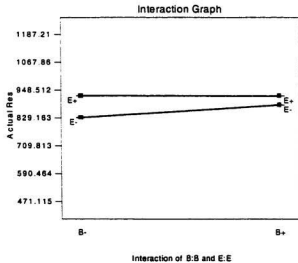


Fig. 6.9 Relationship Between Parameters B and E

Parameter E has high positive effect on the response of the process. Parameter B also has a high positive effect on the response of the process. However as shown in Fig. 6.9, the interaction of these parameters BE, has a high negative effect. Here, the increase of parameter E, while increasing parameter B will cause the decrease of the process' yield. Fig. 6.10 which shows the three-dimensional graph of the relationship among parameters B, E, and the response, indicates that the optimum is achieved when the both parameters B and E are set to the low level. The values are approximately 150 and 180 for B and E, respectively.

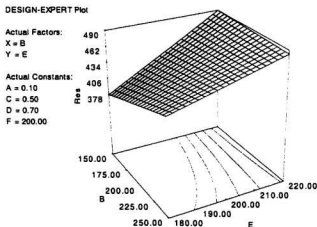


Fig. 6.10 Three-dimensional graph of the relationship among parameters B, E, and the yield of the process

Parameters C and E

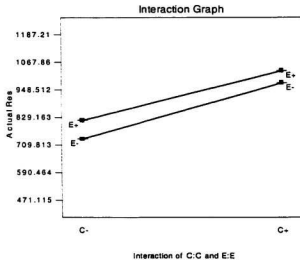


Fig. 6.11 Relationship Between Parameters C and E

Both parameters C and E have the same positive effects but their interaction has a negative effect. Therefore, to reduce the yield of the process, it is better to decrease both parameters. Fig. 6.12 shows the three-dimensional graph of the relationship among parameters C, E, and the response. It shows that the minimum yield of the process is achieved when the value of parameter C is between 0.42 and 0.52 and the value of parameter E is set in the low-level, 180.

DESIGN-EXPERT Plot

Actual Factors:

X = C

Y = E

Actual Constants:

A = 0.10

B = 200.00

D = 0.70

F = 200.00

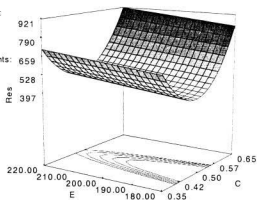


Fig. 6.12 Three-dimensional graph of the relationship among parameters C, E, and the response

Parameters D and E

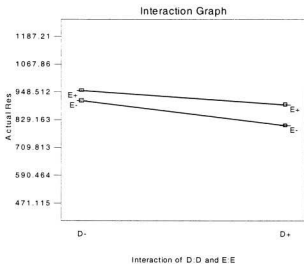


Fig. 6.13 Relationship Between Parameters D and E

Parameter D has high negative effect and parameter E has high positive effect. However, their interaction, DE has a high positive effect on the response of the process. Therefore, an increase of parameter D and decrease of parameter E will decrease the yield of the process. Figure 6.14 shows the three-dimensional graph of the relationship among parameters D, E, and the response. It shows that the effect of the interaction between D and E in fact affects the location of prediction region. The optimum process is achieved when parameter D is set between 0.72 and 0.80, and parameter E is set in the low-level, 180.

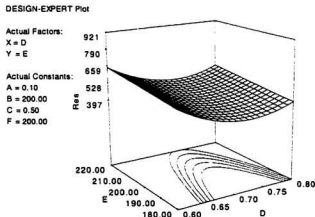


Fig. 6.14 Three-dimensional graph of the relationship among parameters D, E, and the yield of the process

Effects of parameters and their interactions can also be clearly distinguished using a normal plot view shown below.

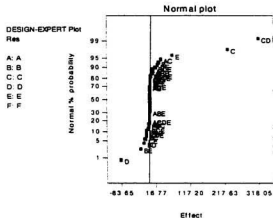


Fig. 6.15 The Normal Plot of Effects

Fig. 6.15 shows parameters C, D, E, and interaction CD lying far away from the normal line. Therefore, C, D, E, and interaction CD are considered to have high effects to the process.

The effect estimations have given some insights into how the various parameters interact and how they can be adjusted to achieve the desired objective. In addition, plots of parameters C and D are seen very curved or steep in the Perturbation plot in Fig 6.15, which were constructed based on the response of sum of absolute residuals, $|E|$. Therefore, parameters C and D are considered to highly affect to the differences between observed and simulated runoffs using the Mock model. This consideration is confirmed by other perturbation plots shown in Appendix D, Figs. D.1, and D. 2, which are constructed based on R^2 , and Dv , respectively.

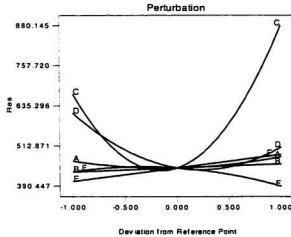


Fig. 6.16 The Perturbation Plot of the Mock Model-Parameters Based on Residuals

6.2. Minimum Required Number of Experiments

For efficiency and cost effectiveness, the minimum number of experiments that will give a comparable fit of the significant polynomial model must be explored. The minimum required number based on manual, CCD, and BBD calibrations are compared for the case of six parameters:

Manual calibration: (uncertain) = 112 experiments used here.

CCD full: (2^6) main + (2×6) augmented + 1 central point = 77 experiments

CCD Res. VI: (2^5) main + (2×6) augmented + 1 central point = 45 experiments

BBD: (2^5) main + (2^4) augmented + 1 central point = 49 experiments

BBD requires fewer experiments than a Full CCD. However, CCD resolution VI for 6 parameters requires fewer experiments than BBD. However, having the information of the minimum number of experiments cannot guarantee the most accurate calibration. Analysis of the polynomial models and verifications of the calibrated model must be conducted to prove that one method of calibration is indeed producing the best results.

6.3. Analysis of Polynomial Models

The significance of the polynomial models, which can fit the response, is identified using lack-of-fit tests. The results, shown in Tables 6.2 and 6.3 are used to examine the best model that can fit the response. CCD and BBD gave similar results. Therefore, only the results of CCD are shown in the examination of the best model.

Table 6.2 ANOVA Table for the CCD Model

| Source | Sum of Squares | DF | Mean Square | F Value | p-value |
|-----------|----------------|----|-------------|---------|----------|
| Mean | 22144100 | 1 | 22144100 | | |
| Linear | 385721 | 6 | 64286.8 | 1.9165 | 0.0978 |
| Quadratic | 1544720 | 21 | 73558.2 | 60.0704 | < 0.0001 |
| Residual | 31837.8 | 26 | 1224.53 | | |
| Total | 24106400 | 54 | 446415 | | |

Table 6.2 shows that a linear model is not appropriate because p-value (0.0978) is not statistically significant at the 5% level. Therefore, response prediction using a linear model can be ruled out. For the quadratic model however, the p-value is less than 0.0001 indicating a statistically significant result. The model is thus identified as a quadratic model. The results in Table 6.3 test the lack-of-fit of the quadratic model against linear model.

Table 6.3 ANOVA Table for Lack-of-Fit Tests for the CCD Model

| | Root | | Adjusted | Predicted | |
|-----------|---------|-----------|-----------|-----------|---------|
| Source | MSE | R-Squared | R-Squared | R-Squared | PRESS |
| Linear | 183.15 | 0.196568 | 0.094002 | 0.05644 | 2073040 |
| Quadratic | 34.9933 | 0.983775 | 0.966926 | 0.915233 | 166336 |

The examination is about focusing on the model to minimise the "PRESS" or equivalently to maximise the "Prediction R-Squares". PRESS stands for the prediction sum of squares. Table 6.3 shows that the quadratic model is superior against the linear model. The quadratic model gave a "PRESS" of 166336 and a "Prediction R-Square" of 0.915233. These results are superior compared to that of the linear model.

After finding out the order of the polynomial model, the next task is to obtain the coefficients for each parameter in the model. Both CCD and BBD will develop their own quadratic model. Based on the t-test statistics, only parameters C, D, E, and their interactions are selected by CCD to establish the quadratic model shown in Table 6.4. On the other hand, all parameters:

A, B, C, D, E, F, and their interactions, shown in Table 6.5, are selected by BBD to establish the quadratic model.

Analysis of the second-order polynomial model developed using CCD

Table 6.4 ANOVA Table of the Coefficients of Polynomial Model developed using CCD Based on 4-Years of Calibration Data

| | Coefficient | | Standard | t for H0 | | |
|----------------|-------------|----|----------|-----------|-----------|---------|
| Factor | Estimate | DF | Error | Coeff=0 | Prob > t | VIF |
| Intercept | 488.678 | 1 | 10.4179 | | | |
| A-A | 7.18915 | 1 | 6.5122 | 0.93296 | 0.318 | 1 |
| B-B | 12.32 | 1 | 6.5122 | 1.07018 | 0.0881 | 1 |
| C-C | 105.3828 | 1 | 6.5122 | 8.19853 | < 0.0001 | 1 |
| D-D | -51.79274 | 1 | 6.5122 | -0.503185 | < 0.0002 | 1 |
| E-E | 40.2711 | 1 | 6.5122 | 2.62949 | < 0.0003 | 1 |
| F-F | -22.6462 | 1 | 6.5122 | -0.403591 | 0.0077 | 1 |
| A ² | 26.79206 | 1 | 9.63472 | 0.704957 | 0.0083 | 1.02947 |
| C ² | 328.253 | 1 | 9.63472 | 30.02 | < 0.0001 | 1.02947 |
| D ² | 114.79 | 1 | 9.63472 | 13.99 | < 0.0001 | 1.02947 |
| F ² | -31.11549 | 1 | 9.63472 | 0.115778 | 0.0082 | 1.02947 |
| AC | 20.993 | 1 | 12.871 | 1.24256 | 0.0181 | 1 |
| BE | -13.6407 | 1 | 12.871 | -1.0598 | 0.0928 | 1 |
| CD | 159.025 | 1 | 12.871 | 12.3553 | < 0.0001 | 1 |

Table 6.4 shows that, although the parameters A, B, and interaction parameters BE are not statistically significant at the 5% level, they must be recruited into the model in order to obey the principle of hierarchy. Single parameters C, D, and F are statistically significant for the linear and quadratic coefficients. Almost all VIF of the coefficients are one, except VIF of quadratic coefficients, 1.02947. Moreover, they are symmetric and orthogonal. Therefore, these indicate no multicollinearity problem occurs in the polynomial model and the region of stationary point is inside the orthogonal

polynomial. The ability to fit the response of the polynomial model can be analysed using ANOVA table below

Table 6.5 ANOVA Table of the Polynomial Model to fit the Response
developed using CCD Based on 4-Years of Calibration Data

| | Sum of | | Mean | F | |
|-------------|---------|----|--|----------|----------|
| Source | Squares | DF | Square | Value | Prob > F |
| Model | 7972540 | 13 | 613272 | 157.8429 | < 0.0001 |
| Residual | 763371 | 38 | 902.4 | | |
| Lack of Fit | 763371 | 33 | 1017.3 | 63660000 | < 0.0001 |
| Pure Error | 0 | 5 | 0 | | |
| Cor Total | 8735910 | 51 | $\lambda_A = \lambda_B = \lambda_C = \lambda_D = \lambda_E = \lambda_F = 1.00$ | | |
| Root MSE | 102.968 | | R-Squared | 0.9781 | |

Table 6.5 shows that the residuals of the polynomial model are linear and therefore, if the residuals are equally spread along the data, the polynomial model provides a good fit to the response. In addition, all eigenvalues, λ_k are approximately equal to one. It means that the optimum value of the response is inside the orthogonal polynomial and the optimisation is to minimise the polynomial model. The quadratic model formed by CCD is then:

$$\begin{aligned}
 Y = & 488.678 + 7.18915 A + 12.32 B + 105.3828 C \\
 & - 51.79274 D + 40.2711 E - 22.6462 F + 26.79206 A^2 \\
 & + 328.253 C^2 + 114.79 D^2 - 31.11549 F^2 + 20.993 AC \\
 & - 13.6407 BE + 159.025 CD
 \end{aligned}
 \tag{6.1}$$

where:

Y = Response (Sum of absolute residuals)

A = Parameter of Coefficient of Impermeable Layer

B = Parameter of Initial Storage Value

C = Parameter of Coefficient of Infiltration

D = Parameter of Coefficient of Recession

E = Parameter of Soil Moisture Capacity

F = Parameter of Initial Soil Moisture

A² = Quadratic-Parameter of Impermeable Layer

C² = Quadratic-Parameter of Coefficient of Infiltration

D² = Quadratic-Parameter of Coefficient of Recession

F² = Quadratic-Parameter of Initial Soil Moisture

AC = Interaction Between Parameters Coefficient of Impermeable Layer (A)
and Coefficient of Infiltration (C)

BE = Interaction Between Parameters Coefficient of Initial Storage Value (B)
and Coefficient of Soil Moisture Capacity (E)

CD = Interaction Between Parameters Coefficient of Infiltration (C) and
Coefficient of Recession (D)

Analysis of the second-order polynomial model developed using BBD

Table 6.6 ANOVA Table of the Coefficients of Polynomial Model developed using BBD Based on 4-Years of Calibration Data

| | Coefficient | | Standard | t for H0 | | |
|----------------|-------------|----|----------|----------|-----------|---------|
| Factor | Estimate | DF | Error | Coeff=0 | Prob > t | VIF |
| Intercept | 446.14 | 1 | 9.41892 | | | |
| A-A | 6.76013 | 1 | 6.89394 | 0.98059 | 0.3327 | 1 |
| B-B | 12.2365 | 1 | 6.89394 | 1.77496 | 0.0835 | 1 |
| C-C | 105.193 | 1 | 6.89394 | 15.2587 | < 0.0001 | 1 |
| D-D | -51.4581 | 1 | 6.89394 | -7.46424 | < 0.0001 | 1 |
| E-E | 40.8853 | 1 | 6.89394 | 5.93061 | < 0.0001 | 1 |
| F-F | -22.1624 | 1 | 6.89394 | -3.21476 | 0.0026 | 1 |
| A ² | 27.2969 | 1 | 10.2254 | 2.66952 | 0.0109 | 1.22222 |
| C ² | 328.812 | 1 | 10.2254 | 32.1565 | < 0.0001 | 1.22222 |
| D ² | 114.445 | 1 | 10.2254 | 11.1922 | < 0.0001 | 1.22222 |
| F ² | -33.5313 | 1 | 10.2254 | -3.27923 | 0.0022 | 1.22222 |
| AC | 21.2552 | 1 | 11.9407 | 1.78007 | 0.0827 | 1 |
| BE | -15.2595 | 1 | 8.44332 | -1.80728 | 0.0782 | 1 |
| CD | 154.099 | 1 | 11.9407 | 12.9054 | < 0.0001 | 1 |

For the BBD, single-parameters A and B, and interactions AC and BE are indicated to have p-values equal 0.3327, 0.0835, 0.0827, and 0.0782, respectively. Therefore, they are considered statistically insignificant at the 5% level. Nevertheless, according to the principle of hierarchy, they must be included into the model. BBD gives a similar model to the model produced by CCD. Both BBD and CCD agree on the single-parameters C, D, E, quadratic-parameters C, D, and interaction CD as the main consideration on building the respective models. Almost all VIF of the coefficients are one, except VIF of quadratic coefficients, 1.22222. Moreover, they are symmetric and orthogonal, which indicates no multicollinearity problem occurs in the polynomial model and the region of stationary point is inside the orthogonal

polynomial. The ability to fit the response of the polynomial model can be analysed using ANOVA table below

Table 6.7 ANOVA Table of the Polynomial Model to fit the Response developed using BBD Based on 4-Years of Calibration Data

| | Sum of | | Mean | F | |
|-------------|---------|----|--|----------|----------|
| Source | Squares | DF | Square | Value | Prob > F |
| Model | 1916650 | 13 | 147435 | 129.257 | < 0.0001 |
| Residual | 45625.4 | 40 | 1140.64 | | |
| Lack of Fit | 45625.4 | 35 | 1303.58 | 63660000 | < 0.0001 |
| Pure Error | 0 | 5 | 0 | | |
| Cor Total | 1962280 | 53 | $\lambda_A = \lambda_B = \lambda_C = \lambda_D = \lambda_E = \lambda_F = 1.00$ | | |
| Root MSE | 33.7733 | | R-Squared | 0.9767 | |

Table 6.7 shows that R-Squares of the polynomial model is 0.9767. Therefore, the polynomial model can really fit the response. In addition, all eigenvalues are also equal to one. It means that the optimum value of the response is inside the orthogonal polynomial and the optimisation is to minimise the polynomial model. The quadratic model formed by BBD is:

$$\begin{aligned}
 Y = & 446.14 + 6.76013 A + 12.2365 B + 105.193 C \\
 & - 51.4581 D + 40.8853 E - 22.1624 F + 27.2969 A^2 \\
 & + 328.812 C^2 + 114.445 D^2 - 33.5313 F^2 + 21.2552 AC \\
 & - 15.2595 BE + 154.099 CD
 \end{aligned} \tag{6.2}$$

where:

Y = Response Data (Sum of absolute residuals)

A = Parameter of Coefficient of Impermeable Layer

B = Parameter of Initial Storage Value

C = Single-Parameter of Coefficient of Infiltration

D = Single-Parameter of Coefficient of Recession

E = Single-Parameter of Soil Moisture Capacity

F = Single-Parameter of Initial Soil Moisture

A² = Quadratic-Parameter of Coefficient of Impermeable Layer

C² = Quadratic-Parameter of Coefficient of Infiltration

D² = Quadratic-Parameter of Coefficient of Recession

F² = Quadratic-Parameter of Initial Soil Moisture

AC = Interaction Between Parameters of Coefficient of Impermeable Layer and Initial Storage Value

BE = Interaction Between Parameters of Initial Storage Value And Soil Moisture Capacity

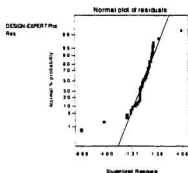
CD = Interaction between Parameters of Coefficient of Infiltration And Coefficient of Recession

After building these two second-order (quadratic) polynomial models, the models must be examined to ensure the models can significantly fit the response and the assumptions of regression are not violated. This examination can be done by the inspection of various plots of the model-

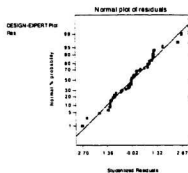
residuals shown in Fig. 6.17, Fig 6.18, and Fig 6.19. Here, the results of CCD will be compared against the results of BBD.

Figure 6.17 shows the normal probability plot of the studentized residuals. Fig. 6.18 shows the outlier-T plot between the run numbers and the outliers-T. Fig. 6.19 shows the leverage plot between the run numbers and the leverages.

Normal Plots



(a) BBD

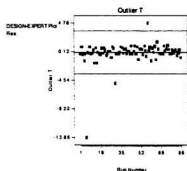


(b) CCD

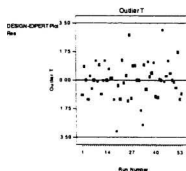
Fig. 6.17 Normal Plots of Studentized Residuals

In Fig. 6.17, both (a) and (b) graphically show that model-residuals produced by CCD are approximately normally distributed. However, the residuals for BBD are not normally distributed.

Outlier-T Plots



(a) BBD

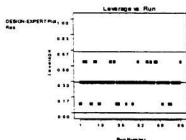


(b) CCD

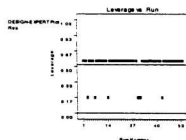
Fig. 6.18 Outlier-T Plots for CCD and BBD

From the plots in Fig. 6.18, the polynomial model established by BBD produces three outlier-points, shown as the three points lying outside the boundary. However, since the number of data points is 49, the three outlier-points are not considered unusual. Fig. 6.18 (b) shows that the polynomial model established by CCD does not produce any outlier-point.

Leverage Plots



(a) BBD



(b) CCD

Fig. 6.19 Leverage Plots for BBD and CCD

From Fig. 6.19, there no outliers are produced by both BBD and CCD. All the data points are within the bands. Therefore, it can be concluded that the models obtained from both BBD and CCD are equally valid. No assumptions of regression were violated except for the normality of the residuals from the BBD.

6.4. Calibrated Model Parameters and Model Verifications

The performances of RSM, which uses CCD and BBD, are compared to the performance of the Trial and Error Method. Here, the first priority objective is to minimise $|E|$, then to maximise R^2 , and finally to minimise D_v . The $|E|$ will be analysed first. If the results of $|E|$ are the same, then R^2 will be used to determine the best result. This analysis strategy will be continued to the third and fourth priority objectives if the results of the first and the second priority objectives produce equal results. Tables 6.8, 6.9, 6.10, and 6.11 present the results of calibrations and verifications based on the various years of available calibration data.

**Table 6.8 The Results of Calibrations Based On One-Year (1973) Data And
The Verifications Based On the Years of 1977 and 1978**

| Calibration of 1 year data (1973) | | | | | | |
|-----------------------------------|-------------|--------------|-------------|--------------|-------------|--------------|
| Items | TE | | BBD | | CCD | |
| A | 0.109 | | 0.1 | | 0.09 | |
| B | 150 | | 166.17 | | 150 | |
| C | 0.48 | | 0.41 | | 0.46 | |
| D | 0.741 | | 0.8 | | 0.73 | |
| E | 190 | | 180 | | 180 | |
| F | 190 | | 210 | | 210 | |
| | Calibration | Verification | Calibration | Verification | Calibration | Verification |
| /E/ | 30.1389 | 54.55705 | 40.9926 | 52.7216 | 27.919 | 47.2333 |
| R ² | 0.9966 | 0.988681 | 0.9958 | 0.9891 | 0.9978 | 0.9899 |
| Dv | 0.4812 | 0.5984 | 0.4658 | 0.494 | 0.4531 | 0.4772 |

- Appendix D Tables D. 4 and D. 7 show The Polynomial Models developed using CCD and BBD, respectively based on 1-Year Calibration Data.

Table 6.8 shows that generally, Trial and Error, BBD, and CCD gave similar results. However, the /E/ produced by CCD, 27.919 is the smallest. It means that for one-year data calibration, 1973, CCD produces the best results. This is also confirmed by the highest of R², 0.9978. Further, the results of verification also showed that CCD produces the best results. The results of the one-year data for calibration are then compared to two-year, three-year, and four-year of available data for calibration.

Table 6.9 presents the results of calibration and verification based on two years of data.

Table 6.9 Results of Calibrations Based On Two-Years (1973 and 1974) Data
and The Verifications Based On the Years of 1977 and 1978

| Calibration of 2 years data (1973 and 1974) | | | | | | |
|---|-------------|--------------|-------------|--------------|-------------|--------------|
| Items | TE | | BBD | | CCD | |
| A | 0.12 | | 0.10 | | 0.11 | |
| B | 150 | | 150 | | 150 | |
| C | 0.508 | | 0.450 | | 0.460 | |
| D | 0.715 | | 0.760 | | 0.760 | |
| E | 187.854 | | 180.020 | | 180.000 | |
| F | 190 | | 210 | | 190 | |
| | Calibration | Verification | Calibration | Verification | Calibration | Verification |
| Res | 128.4568 | 175.6574 | 91.1368 | 108.9525 | 90.5997 | 106.8744 |
| R ² | 0.9938 | 0.9888 | 0.9976 | 0.9952 | 0.9977 | 0.9950 |
| Dv | 0.6716 | 0.6749 | 0.2386 | 0.3721 | 0.2329 | 0.3953 |

- Appendix D Tables D. 4 and D. 7 show The Polynomial Models developed using CCD and BBD, respectively based on 2 Years Calibration Data.

The analysis of goodness-of-fit for two-year data calibrations showed that the CCD gave the best results. Here, CCD produces the smallest /E/, the highest of R², and the closest to zero of RME, although Dv does not show the best result. This conclusion is also shown by the results of verifications. The results of verifications showed that the performance of CCD is the best because it gave the smallest /E/, the highest R², and the smallest Dv. The results of BBD are second best although the results of BBD are very close to the results of CCD. The results of Trial and Error show are quite different from the results of the BBD or CCD. Table 6.10 presents the results of calibrations and verifications based on three years of available data.

Table 6.10 Results of Calibrations Based On Three-Years (1973, 1974, and 1975) Data and The Verifications Based On the Years of 1977 and 1978

| Calibration of 3 year data (1973, 1974, and 1975) | | | | | | |
|---|-------------|--------------|-------------|--------------|-------------|--------------|
| Items | TE | | BBD | | CCD | |
| A | 0.12 | | 0.1 | | 0.09 | |
| B | 150 | | 150.32 | | 150 | |
| C | 0.521 | | 0.45 | | 0.46 | |
| D | 0.71 | | 0.76 | | 0.74 | |
| E | 186.015 | | 180.02 | | 180.01 | |
| F | 190 | | 210 | | 210 | |
| | Calibration | Verification | Calibration | Verification | Calibration | Verification |
| Res | 200.3141 | 213.9945 | 107.9525 | 143.9203 | 107.2714 | 143.1942 |
| R ² | 0.992 | 0.988293 | 0.9978 | 0.9948 | 0.9979 | 0.9949 |
| Dv | 0.4658 | 0.218837 | 0.3721 | 0.2446 | 0.3161 | 0.2422 |

- Appendix D Tables D. 5 and D. 8 show The Polynomial Models developed using CCD and BBD, respectively based on 3 Years Calibration Data.

Table 6.10 shows either BBD or CCD can be used since they produced similar results. Based on three years of data (1973, 1974, and 1975) for calibration, CCD gave the best results for calibration and verification. It gave the smallest of /E/ and the highest of R².

Table 6.11 shows the results of calibrations based on four available years of data for calibration and the verifications.

Table 6.11 Results of Calibrations Based On Four-Years (1973, 1974, 1975, and 1976) Data and The Verifications

| Calibration of 4-year data (1973, 1974, 1975, and 1976) | | | | | | |
|---|-------------|--------------|-------------|--------------|-------------|--------------|
| Items | TE | | BBD | | CCD | |
| A | 0.12 | | 0.10 | | 0.10 | |
| B | 150.0 | | 150.6 | | 150.0 | |
| C | 0.53 | | 0.45 | | 0.43 | |
| D | 0.70 | | 0.75 | | 0.77 | |
| E | 180 | | 180 | | 180 | |
| F | 190 | | 197 | | 197.3 | |
| | Calibration | Verification | Calibration | Verification | Calibration | Verification |
| Res | 213.978 | 389.0252 | 101.5705 | 233.9174 | 99.8054 | 223.1259 |
| R ² | 0.9907 | 0.985322 | 0.9981 | 0.9978 | 0.9989 | 0.9982 |
| Dv | 0.3587 | 0.36683 | 0.3316 | 0.3522 | 0.3067 | 0.3233 |

For four years of calibration data, CCD gave the best results. It gave the smallest of $/E/$, 99.8054 and the highest of R^2 , 0.9989. Similarly for the verifications, CCD gave the smallest of $/E/$, 223.1259, the highest of R^2 , 0.9982, and the smallest of Dv, 0.3233. These results are also the best compared to those with less than four years of data for calibration. It shows that the longer the available data for calibration, the better the results.

Fig. 6.20 and Fig. 6.21 show the plots of the simulated and observed runoffs during the calibration and verification periods, respectively.

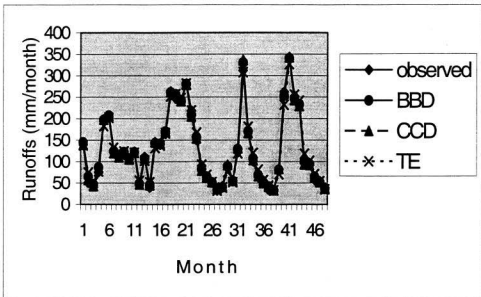


Fig. 6.20 Observed and Simulated Runoffs for Calibration

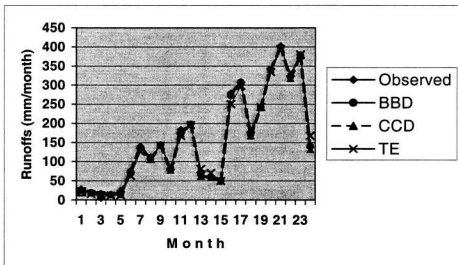


Fig.6.21 Observed and Simulated Runoffs for Verification

Fig.6.20 and Fig.6.21 show that simulated runoffs that are generated using parameters, which are calibrated by both CCD and BBD, provide good fit to the observed runoffs. The results have proved that CCD and BBD are good methods to calibrate rainfall-runoff models. Since both can obtain calibrated parameters, which can be used in the Mock model to produce simulated runoffs that are very similar to the observed runoffs. The final calibrated parameters based on BBD are shown in Table 6.10. The matches between simulated and observed runoffs for the calibration and verification are clearly shown in Fig. 6. 22 and Fig.6. 23.

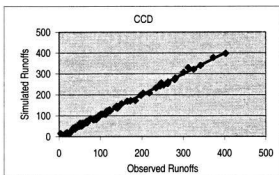


Fig. 6.22.a The Plot of Simulated and Observed Runoffs for Calibration based on CCD

Fig. 6.22.a shows that the plot of observed and simulated runoffs is linear. All points lay on the line of the plot. It means that simulated runoffs based on CCD for the calibration fit the observed runoffs.

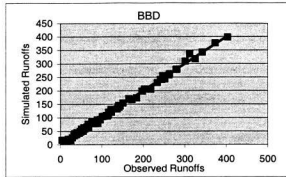


Fig. 6.22.b The Plot of Simulated and Observed Runoffs for Calibration based on BBD

Fig. 6.22.b shows that the plot of observed and simulated runoffs is linear. Almost all points lie on the line of the plot. Only one point is plotted out from the line. It means that simulated runoffs based on BBD for the calibration also fit the observed runoffs, although it is not as good as CCD.

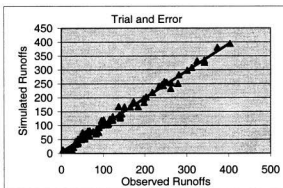


Fig. 6.22.c The Plot of Simulated and Observed Runoffs for Calibration based on Trial and Error

Fig. 6.22.c shows that the plot of observed and simulated runoffs is linear with some points lie outside the line of the plot. It means that simulated runoffs based on Trial and Error for the calibration is the worst fit the observed runoffs compared to the CCD and BBD.

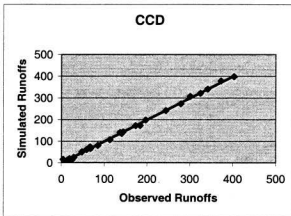


Fig. 6.23.a The Plot of Simulated and Observed Runoffs for Verification based on CCD

Fig. 6.23.a shows that the plot of observed and simulated runoffs in the verification is linear. All points lay on the line of the plot. It means that simulated runoffs based on CCD for the verification fit the observed runoffs.

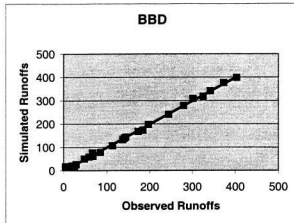


Fig. 6.23.b The Plot of Simulated and Observed Runoffs for Verification based on BBD

Fig. 6.23.b shows that the plot of observed and simulated runoffs in the verification based on BBD is linear. Almost all points lay on the line of the plot. It means that simulated runoffs based on BBD for the verification also fit the observed runoffs. However, it is not as good as CCD.

Next, Fig. 6.22.c shows that the plot of observed and simulated runoffs is linear, with some points off the line of the plot. It means that although the fit of simulated runoffs based on Trial and Error for the calibration is accepted; it is however, the worst fit compared to the CCD and BBD.

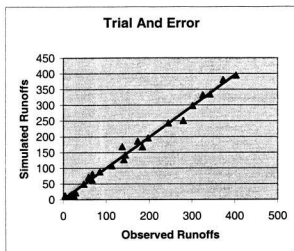


Fig.6.23.c The Plot of Simulated and Observed Runoffs for Verification based on Trial And Error

Table 6.12 The Calibrated Parameters of Mock Rainfall-Runoff Model Based on Four Years (1973 to 1976) Data Using CCD

| Parameters | | Code | Units | Values |
|----------------------------|--------|------|-------|--------|
| % of Impermeable Layer | IMLA | A | - | 0.10 |
| Initial Storage Value | V_0 | B | mm | 150.0 |
| Coeff. of Infiltration | COI | C | - | 0.43 |
| Monthly Coef. of Recession | K | D | - | 0.77 |
| Soil Moisture Capacity | SMC | E | mm | 180 |
| Initial Soil Moisture | SM_0 | F | mm | 197.3 |

As can be seen from Tables 6.8 to 6.12, the calibrated values of the parameters of the Mock model changes each time additional data becomes

available for calibration. The longer the period available for calibration will always give better results and will give results that are more representative of the basin over an extended period.

Chapter 7

Conclusions

The previous chapters have demonstrated the application of the well-known techniques of experimental design (DOE) and subsequent Response Surface Methodology (RSM) in calibrating a rainfall-runoff model. These techniques are commonly used in industrial experimentation for product or process improvements. The DOE-RSM approach provides a systematic way of learning about the importance of each parameter in the model and more importantly how they interact with one another. Then, using this knowledge a simple quadratic regression type equation can be developed to model the resulting response of the process or model. The values of the parameters that optimises (minimise or maximise) the response can then be found. Another advantage of this approach is that standard statistical software packages such as Minitab, Statistica, SPSS, SAS which has DOE-RSM capability and standard stand-alone DOE-RSM packages such as Design-Expert and Design-Ease, can be used for model calibration. This obviates the need for writing special computer programs as required in other numerical calibration methods or spending endless amount of time in the trial-and-error approach.

In this thesis the Mock rainfall-runoff model, which has six parameters, was calibrated using the DOE-RSM approach. It was shown

that the calibrated model provided a very good fit between observed and simulated data both for the calibration data sets as well as the verification data sets. In general, it can be concluded that the DOE-RSM approach is a viable and excellent alternative for the calibration of the multi-parameter Mock rainfall-runoff model. The following are specific conclusions regarding some of the details in conducting the design of experiments and the application of the Response Surface Methodology in calibrating the Mock model:

1. In the design of experiment phase, either full factorial or fractional factorial designs can be used. It was shown that the Central Composite Design (CCD), which uses a full factorial design or one-half fractional factorial design, and the Box-Benhken Design (BBD) can provide accurate calibration of the Mock rainfall-runoff model using a small number of experiments. Both designs gave similar results.
2. BBD required fewer experiments than the CCD of full version. However, CCD of resolution VI can reduce the number of experiments less than BBD. Moreover, the results of CCD resolution VI are the same as the results of CCD of full version. They are better than BBD, although the results of BBD are close to the results of CCD. Therefore, it is better to use CCD using resolution VI instead of BBD, particularly when there are large number of parameters to calibrate. However, further analysis must be carried out before one can say that one design is better than the other.

The better design is the one that will give a better match between the simulated and observed data.

3. Based on the effect analysis factors B, C, E, A^2 , C^2 , D^2 , AC, and CD have high positive effects on the response of the model, while, D, F, F^2 , BE have high negative effects on the response of the model. It means that to optimise the response of the process, for example: to reduce the absolute sum of errors, modellers have to decrease parameters and interactions that have positive effects and to increase parameters and interactions that have negative effects. Therefore, the parameters, which are considered as the priorities to optimise the process, are recognised. In this research, for these particular data, the single-parameters, which affect very much the change of the Mock model's process are: Coefficient of Infiltration (COI) coded as C, Coefficient of Recession (K) coded as D, and Soil Moisture Capacity (SMC) coded as E. While, only the interaction CD highly affects the Mock model process.

While it was shown in this thesis that the DOE-RSM approach successfully calibrated a model with 6 parameters, it may require more effort when there are a large number of parameters to be calibrated (e.g., more than 10 parameters). In this situation, to keep the number of experiments to a manageable level, one may have to use highly fractional factorial designs which may or may not be desirable because many of the factors will be aliased.

In addition, when calibrating a model without any prior knowledge of the possible ranges of the parameters, it may require major effort simply to determine the workable ranges of each parameter. Then, for a more accurate estimate of the parameters, the ranges must be shortened so that the peak of the response surface is indeed the global optimal.

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APPENDIX A

Computer Program

Appendix A

A Computer Program For the Mock Rainfall-Runoff Model

The quick basic program of Mock model

The Mock model is calculated using a program of quick basic (Kadarisman, 1993). The program is

```
'MOCK MODEL PROGRAM.
'=====
'=====
GOSUB initialization
GOSUB water.balance
GOSUB run.off
END

'=====
initialization:
'=====
CLS
INPUT "impermeable layer (imla)="; imla
INPUT "initial storage (Vo)="; vo
INPUT "coefficient of infiltration (COI)="; coi
INPUT "monthly coefficient recession (K)="; k
INPUT "soil moisture capacity (SMC)="; smc
INPUT "initial soil moisture (SMo)="; smo

LET a = 4: b = 12
DIM p(a, b): DIM ws(a, b): DIM eact(a, b)
DIM ce(a, b): DIM eto(a, b): DIM pe(a, b): DIM a1(a, b): DIM b1(a, b)
DIM inf(a, b): DIM vn(a, b): DIM dltn(a, b): DIM bf(a, b)
DIM dro(a, b): DIM ro(a, b): DIM dsro(a, b): DIM storm(a, b)
DIM qo(a, b): DIM sm(a, b): DIM ss(a, b)
vn(1, 0) = vo:
```

RETURN

=====

water.balance:

=====

CLS

OPEN "a:ro.dat" FOR OUTPUT AS #1

OPEN "a:ws.dat" FOR OUTPUT AS #2

OPEN "a:dsro.dat" FOR OUTPUT AS #3

OPEN "a:eto.dat" FOR INPUT AS #4 'Pot.evapotrans.data

OPEN "a:montkada.dat" FOR INPUT AS #5 'monthly precipitation

OPEN "a:vn.dat" FOR OUTPUT AS #6

FOR y = 1 TO a

FOR m = 1 TO b

INPUT #5, p(y, m)

NEXT m

NEXT y

CLOSE #5

FOR y = 1 TO a

FOR m = 1 TO b

INPUT #4, eto(y, m)

NEXT m

NEXT y

CLOSE #4

FOR y = 1 TO a

FOR m = 1 TO b

IF m = 1 AND y > 1 THEN

sm(y, (m - 1)) = sm((y - 1), b)

ELSEIF m = 1 AND y = 1 THEN

sm(y, (m - 1)) = smo

END IF

'The calculation of water balance

.....

LET eact(y, m) = eto(y, m)

100 eact(y, m) = ce(y, m)

200 pe(y, m) = p(y, m) - eact(y, m)

IF pe(y, m) > 0 THEN

IF sm(y, m - 1) < smc THEN

IF (pe(y, m) + sm(y, (m - 1))) < smc THEN

ss(y, m) = pe(y, m): sm(y, m) = sm(y, (m - 1)) + ss(y, m)

ELSEIF (pe(y, m) + sm(y, (m - 1))) > smc THEN

```

ss(y, m) = smc - sm(y, (m - 1)): sm(y, m) = smc
END IF
ELSEIF sm(y, m - 1) = smc THEN
ss(y, m) = 0: sm(y, m) = sm(y, (m - 1)) + ss(y, m)
END IF
ELSEIF pe(y, m) < 0 THEN
IF sm(y, (m - 1)) = smc THEN
IF (pe(y, m) + sm(y, (m - 1))) < 0 THEN
ss(y, m) = pe(y, m): sm(y, m) = 0
ELSEIF pe(y, m) + sm(y, (m - 1)) > 0 THEN
ss(y, m) = pe(y, m): sm(y, m) = sm(y, (m - 1)) + pe(y, m)
END IF
ELSEIF sm(y, (m - 1)) < smc THEN
IF (pe(y, m) + sm(y, (m - 1))) < 0 THEN
ss(y, m) = pe(y, m): sm(y, m) = 0
ELSEIF (pe(y, m) + sm(y, (m - 1))) > 0 THEN
ss(y, m) = pe(y, m): sm(y, m) = sm(y, (m - 1)) + pe(y, m)
END IF
END IF
END IF

```

```

ce(y, m) = eto(y, m) * sm(y, m) / smc
IF ABS(ce(y, m) - eact(y, m)) > .01 THEN
GOTO 100
ELSEIF ABS(ce(y, m) - eact(y, m)) <= .01 THEN
ws(y, m) = pe(y, m) - ss(y, m)
END IF
PRINT
IF ws(y, m) = 0 THEN
dsro(y, m) = imlia * p(y, m)
sm(y, m) = sm(y, m - 1) + pe(y, m) - dsro(y, m)
IF sm(y, m) > smc THEN
sm(y, m) = smc
ws(y, m) = sm(y, m - 1) + pe(y, m) - dsro(y, m) - smc
ELSEIF sm(y, m) < smc THEN
sm(y, m) = sm(y, m)
END IF
ELSEIF ws(y, m) > 0 THEN
GOTO 300
END IF
300 PRINT
WRITE #2, ws(y, m)
WRITE #3, dsro(y, m)
NEXT m
NEXT y
CLOSE #2: CLOSE #3

```

RETURN

'=====

run.off:

'=====

CLS

'This calculation is based on water balance principle
'and refers to MOCK, (1973). Water Availability Appraisal,
'Report for Land Capability Appraisal, Indonesia.

```
OPEN "a:\ws.dat" FOR INPUT AS #7
OPEN "a:\dsro.dat" FOR INPUT AS #8
FOR y = 1 TO a
  FOR m = 1 TO b
    INPUT #7, ws(y, m): INPUT #8, dsro(y, m):
  NEXT m
NEXT y
CLOSE #7: CLOSE #8:
FOR y = 1 TO a
  FOR m = 1 TO b
    IF m = 1 AND y > 1 THEN
      vn(y, (m - 1)) = vn((y - 1), b)
    END IF
    inf(y, m) = coi * ws(y, m)
    a1(y, m) = .5 * (k + 1) * inf(y, m)
    b1(y, m) = k * vn(y, m - 1)
    vn(y, m) = a1(y, m) + b1(y, m)
    WRITE #6, vn(y, m)
    dltvn(y, m) = vn(y, m) - vn(y, m - 1)
    bf(y, m) = inf(y, m) - dltvn(y, m)
    dro(y, m) = ws(y, m) - inf(y, m)
    storm(y, m) = dsro(y, m)
    ro(y, m) = bf(y, m) + dro(y, m) + storm(y, m)
    WRITE #1, ro(y, m)
  NEXT m
NEXT y
CLOSE #1
RETURN
END
```

Appendix B

Tables of the Arranged Experiments

Table B.1 Table of Experiments Arranged Based On CCD for the Six Parameters

| A | B | C | D | E | F |
|------|-----|------|-----|-----|-----|
| 0.08 | 150 | 0.35 | 0.6 | 180 | 190 |
| 0.12 | 150 | 0.35 | 0.6 | 180 | 190 |
| 0.08 | 250 | 0.35 | 0.6 | 180 | 190 |
| 0.12 | 250 | 0.35 | 0.6 | 180 | 190 |
| 0.08 | 150 | 0.65 | 0.6 | 180 | 190 |
| 0.12 | 150 | 0.65 | 0.6 | 180 | 190 |
| 0.08 | 250 | 0.65 | 0.6 | 180 | 190 |
| 0.12 | 250 | 0.65 | 0.6 | 180 | 190 |
| 0.08 | 150 | 0.35 | 0.8 | 180 | 190 |
| 0.12 | 150 | 0.35 | 0.8 | 180 | 190 |
| 0.08 | 250 | 0.35 | 0.8 | 180 | 190 |
| 0.12 | 250 | 0.35 | 0.8 | 180 | 190 |
| 0.08 | 150 | 0.65 | 0.8 | 180 | 190 |
| 0.12 | 150 | 0.65 | 0.8 | 180 | 190 |
| 0.08 | 250 | 0.65 | 0.8 | 180 | 190 |
| 0.12 | 250 | 0.65 | 0.8 | 180 | 190 |
| 0.08 | 150 | 0.35 | 0.6 | 220 | 190 |
| 0.12 | 150 | 0.35 | 0.6 | 220 | 190 |
| 0.08 | 250 | 0.35 | 0.6 | 220 | 190 |
| 0.12 | 250 | 0.35 | 0.6 | 220 | 190 |
| 0.08 | 150 | 0.65 | 0.6 | 220 | 190 |
| 0.12 | 150 | 0.65 | 0.6 | 220 | 190 |
| 0.08 | 250 | 0.65 | 0.6 | 220 | 190 |
| 0.12 | 250 | 0.65 | 0.6 | 220 | 190 |
| 0.08 | 150 | 0.35 | 0.8 | 220 | 190 |
| 0.12 | 150 | 0.35 | 0.8 | 220 | 190 |
| 0.08 | 250 | 0.35 | 0.8 | 220 | 190 |
| 0.12 | 250 | 0.35 | 0.8 | 220 | 190 |
| 0.08 | 150 | 0.65 | 0.8 | 220 | 190 |
| 0.12 | 150 | 0.65 | 0.8 | 220 | 190 |
| 0.08 | 250 | 0.65 | 0.8 | 220 | 190 |
| 0.12 | 250 | 0.65 | 0.8 | 220 | 190 |
| 0.08 | 150 | 0.35 | 0.6 | 180 | 210 |
| 0.12 | 150 | 0.35 | 0.6 | 180 | 210 |
| 0.08 | 250 | 0.35 | 0.6 | 180 | 210 |
| 0.12 | 250 | 0.35 | 0.6 | 180 | 210 |
| 0.08 | 150 | 0.65 | 0.6 | 180 | 210 |
| 0.12 | 150 | 0.65 | 0.6 | 180 | 210 |
| 0.08 | 250 | 0.65 | 0.6 | 180 | 210 |
| 0.12 | 250 | 0.65 | 0.6 | 180 | 210 |

| | | | | | |
|----------|---------|----------|----------|---------|---------|
| 0.08 | 150 | 0.35 | 0.8 | 180 | 210 |
| 0.12 | 150 | 0.35 | 0.8 | 180 | 210 |
| 0.08 | 250 | 0.35 | 0.8 | 180 | 210 |
| 0.12 | 250 | 0.35 | 0.8 | 180 | 210 |
| 0.08 | 150 | 0.65 | 0.8 | 180 | 210 |
| 0.12 | 150 | 0.65 | 0.8 | 180 | 210 |
| 0.08 | 250 | 0.65 | 0.8 | 180 | 210 |
| 0.12 | 250 | 0.65 | 0.8 | 180 | 210 |
| 0.08 | 150 | 0.35 | 0.6 | 220 | 210 |
| 0.12 | 150 | 0.35 | 0.6 | 220 | 210 |
| 0.08 | 250 | 0.35 | 0.6 | 220 | 210 |
| 0.12 | 250 | 0.35 | 0.6 | 220 | 210 |
| 0.08 | 150 | 0.65 | 0.6 | 220 | 210 |
| 0.12 | 150 | 0.65 | 0.6 | 220 | 210 |
| 0.08 | 250 | 0.65 | 0.6 | 220 | 210 |
| 0.12 | 250 | 0.65 | 0.6 | 220 | 210 |
| 0.08 | 150 | 0.35 | 0.8 | 220 | 210 |
| 0.12 | 150 | 0.35 | 0.8 | 220 | 210 |
| 0.08 | 250 | 0.35 | 0.8 | 220 | 210 |
| 0.12 | 250 | 0.35 | 0.8 | 220 | 210 |
| 0.08 | 150 | 0.65 | 0.8 | 220 | 210 |
| 0.12 | 150 | 0.65 | 0.8 | 220 | 210 |
| 0.08 | 250 | 0.65 | 0.8 | 220 | 210 |
| 0.12 | 250 | 0.65 | 0.8 | 220 | 210 |
| 0.043432 | 200 | 0.5 | 0.7 | 200 | 200 |
| 0.156569 | 200 | 0.5 | 0.7 | 200 | 200 |
| 0.1 | 58.5786 | 0.5 | 0.7 | 200 | 200 |
| 0.1 | 341.421 | 0.5 | 0.7 | 200 | 200 |
| 0.1 | 200 | 0.075736 | 0.7 | 200 | 200 |
| 0.1 | 200 | 0.924264 | 0.7 | 200 | 200 |
| 0.1 | 200 | 0.5 | 0.417157 | 200 | 200 |
| 0.1 | 200 | 0.5 | 0.982843 | 200 | 200 |
| 0.1 | 200 | 0.5 | 0.7 | 143.431 | 200 |
| 0.1 | 200 | 0.5 | 0.7 | 256.569 | 200 |
| 0.1 | 200 | 0.5 | 0.7 | 200 | 171.716 |
| 0.1 | 200 | 0.5 | 0.7 | 200 | 228.284 |
| 0.1 | 200 | 0.5 | 0.7 | 200 | 200 |
| 0.1 | 200 | 0.5 | 0.7 | 200 | 200 |
| 0.1 | 200 | 0.5 | 0.7 | 200 | 200 |
| 0.1 | 200 | 0.5 | 0.7 | 200 | 200 |
| 0.1 | 200 | 0.5 | 0.7 | 200 | 200 |
| 0.1 | 200 | 0.5 | 0.7 | 200 | 200 |
| 0.1 | 200 | 0.5 | 0.7 | 200 | 200 |

| | | | | | |
|-----|-----|-----|-----|-----|-----|
| 0.1 | 200 | 0.5 | 0.7 | 200 | 200 |
| 0.1 | 200 | 0.5 | 0.7 | 200 | 200 |

Table B.2 Table of Experiments Arranged Based On BBD for the Six Parameters

| A | B | C | D | E | F |
|------|-----|------|-----|-----|-----|
| 0.08 | 150 | 0.5 | 0.6 | 200 | 200 |
| 0.12 | 150 | 0.5 | 0.6 | 200 | 200 |
| 0.08 | 250 | 0.5 | 0.6 | 200 | 200 |
| 0.12 | 250 | 0.5 | 0.6 | 200 | 200 |
| 0.08 | 150 | 0.5 | 0.8 | 200 | 200 |
| 0.12 | 150 | 0.5 | 0.8 | 200 | 200 |
| 0.08 | 250 | 0.5 | 0.8 | 200 | 200 |
| 0.12 | 250 | 0.5 | 0.8 | 200 | 200 |
| 0.1 | 150 | 0.35 | 0.7 | 180 | 200 |
| 0.1 | 250 | 0.35 | 0.7 | 180 | 200 |
| 0.1 | 150 | 0.65 | 0.7 | 180 | 200 |
| 0.1 | 250 | 0.65 | 0.7 | 180 | 200 |
| 0.1 | 150 | 0.35 | 0.7 | 220 | 200 |
| 0.1 | 250 | 0.35 | 0.7 | 220 | 200 |
| 0.1 | 150 | 0.65 | 0.7 | 220 | 200 |
| 0.1 | 250 | 0.65 | 0.7 | 220 | 200 |
| 0.1 | 200 | 0.35 | 0.6 | 200 | 190 |
| 0.1 | 200 | 0.65 | 0.6 | 200 | 190 |
| 0.1 | 200 | 0.35 | 0.8 | 200 | 190 |
| 0.1 | 200 | 0.65 | 0.8 | 200 | 190 |
| 0.1 | 200 | 0.35 | 0.6 | 200 | 210 |
| 0.1 | 200 | 0.65 | 0.6 | 200 | 210 |
| 0.1 | 200 | 0.35 | 0.8 | 200 | 210 |
| 0.1 | 200 | 0.65 | 0.8 | 200 | 210 |
| 0.08 | 200 | 0.5 | 0.6 | 180 | 200 |
| 0.12 | 200 | 0.5 | 0.6 | 180 | 200 |
| 0.08 | 200 | 0.5 | 0.8 | 180 | 200 |
| 0.12 | 200 | 0.5 | 0.8 | 180 | 200 |
| 0.08 | 200 | 0.5 | 0.6 | 220 | 200 |
| 0.12 | 200 | 0.5 | 0.6 | 220 | 200 |
| 0.08 | 200 | 0.5 | 0.8 | 220 | 200 |
| 0.12 | 200 | 0.5 | 0.8 | 220 | 200 |
| 0.1 | 150 | 0.5 | 0.7 | 180 | 190 |
| 0.1 | 250 | 0.5 | 0.7 | 180 | 190 |

| | | | | | |
|------|-----|------|-----|-----|-----|
| 0.1 | 150 | 0.5 | 0.7 | 220 | 190 |
| 0.1 | 250 | 0.5 | 0.7 | 220 | 190 |
| 0.1 | 150 | 0.5 | 0.7 | 180 | 210 |
| 0.1 | 250 | 0.5 | 0.7 | 180 | 210 |
| 0.1 | 150 | 0.5 | 0.7 | 220 | 210 |
| 0.1 | 250 | 0.5 | 0.7 | 220 | 210 |
| 0.08 | 200 | 0.35 | 0.7 | 200 | 190 |
| 0.12 | 200 | 0.35 | 0.7 | 200 | 190 |
| 0.08 | 200 | 0.65 | 0.7 | 200 | 190 |
| 0.12 | 200 | 0.65 | 0.7 | 200 | 190 |
| 0.08 | 200 | 0.35 | 0.7 | 200 | 210 |
| 0.12 | 200 | 0.35 | 0.7 | 200 | 210 |
| 0.08 | 200 | 0.65 | 0.7 | 200 | 210 |
| 0.12 | 200 | 0.65 | 0.7 | 200 | 210 |
| 0.1 | 200 | 0.5 | 0.7 | 200 | 200 |
| 0.1 | 200 | 0.5 | 0.7 | 200 | 200 |
| 0.1 | 200 | 0.5 | 0.7 | 200 | 200 |
| 0.1 | 200 | 0.5 | 0.7 | 200 | 200 |
| 0.1 | 200 | 0.5 | 0.7 | 200 | 200 |

Appendix C

Sign Tables

Tables C.1 Table Signs For Six Parameters Full Factorial Designs

| | A | B | AB | C | AC | BC | A B C | D | A D | B D | A B D | C D | A C D | B C D | A B C D |
|------|---|---|----|---|----|----|-------------|---|--------|--------|-------------|--------|-------------|-------------|------------------|
| (1) | - | - | + | - | + | + | - | - | + | + | - | + | - | - | + |
| a | + | - | - | - | - | + | + | - | - | + | + | + | + | - | - |
| b | - | + | - | - | - | - | + | - | + | - | + | + | + | + | - |
| ab | + | + | + | - | + | - | - | - | - | - | - | + | - | + | + |
| c | - | - | + | + | + | - | + | - | + | + | - | - | - | + | - |
| ac | + | - | - | + | - | - | - | - | + | + | - | + | + | + | + |
| bc | - | + | - | + | - | + | - | - | + | - | + | - | + | - | + |
| abc | + | + | + | + | + | + | + | - | - | - | - | - | - | - | - |
| d | - | - | + | - | + | + | - | + | - | - | + | - | + | + | - |
| ad | + | - | - | - | - | + | + | + | + | - | - | - | - | + | + |
| bd | - | + | - | - | - | - | + | + | - | + | - | - | - | - | + |
| abd | + | + | + | - | + | - | - | + | + | + | + | + | + | - | - |
| cd | - | - | + | + | + | - | + | + | - | - | + | + | + | - | + |
| acd | + | - | - | + | - | - | - | + | + | - | - | + | - | - | - |
| bcd | - | + | - | + | - | + | - | + | - | + | - | + | - | + | - |
| abcd | + | + | + | + | + | + | + | + | + | + | + | + | + | + | + |

Tables C.1 Table Signs for Six Parameters Full Factorial Designs

(continued)

| | E | A E | B E | A B E | C E | A C E | B C E | A B C E | D E | A D E | B D E | A B D E | C D E | A C D E | B C D E | A B C D E |
|-----|---|--------|--------|-------------|--------|-------------|-------------|------------------|--------|-------------|-------------|------------------|-------------|------------------|------------------|-----------------------|
| (1) | - | + | + | - | + | - | - | + | + | - | - | + | - | + | + | - |
| a | - | - | + | + | + | + | - | - | + | + | - | - | - | - | + | + |
| b | - | + | - | + | + | + | + | - | + | - | + | + | - | - | + | + |
| ab | - | - | - | - | + | - | + | + | + | + | + | + | + | - | - | - |
| c | - | + | + | - | - | + | - | + | - | + | - | + | + | + | - | + |
| ac | - | - | + | + | - | + | + | + | + | + | - | - | + | + | - | - |
| bc | - | + | - | + | - | + | - | + | + | - | + | - | + | + | - | - |
| abc | - | - | - | - | - | - | - | - | + | + | + | + | + | + | + | + |

| | | | | | | | | | | | | | | | | |
|------|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| d | - | + | + | - | + | - | - | + | - | + | + | - | + | - | - | + |
| ad | - | - | + | + | + | + | - | - | - | - | + | + | + | + | - | - |
| bd | - | + | - | + | + | + | + | - | - | + | - | + | + | - | + | - |
| abd | - | - | - | - | + | - | + | + | - | - | - | - | + | + | + | + |
| cd | - | + | + | - | - | - | + | - | - | + | + | - | - | + | + | - |
| acd | - | - | + | + | - | + | + | + | - | - | + | + | - | - | + | + |
| bcd | - | + | - | + | - | + | - | + | - | + | - | + | - | + | - | + |
| abcd | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - |

Tables C.1 Table Signs for Six Parameters Full Factorial Designs

(continued)

| | F | A F | B F | A B F | C F | A C F | B C F | A B C F | D F | A D F | B D F | A B D F | C D F | A C D F | B C D F | A B C D F |
|------|---|--------|--------|-------------|--------|-------------|-------------|------------------|--------|-------------|-------------|------------------|-------------|------------------|------------------|-----------------------|
| (1) | - | + | + | - | + | - | - | + | + | - | - | + | - | + | + | - |
| a | - | - | + | + | + | + | - | - | + | + | - | - | - | - | + | + |
| b | - | + | - | + | + | - | + | - | + | - | + | - | - | - | - | + |
| ab | - | - | - | + | + | + | + | + | + | + | + | + | - | + | - | - |
| c | - | + | + | - | - | + | + | - | + | - | - | + | + | + | - | + |
| ac | - | - | + | + | - | - | + | + | + | + | - | - | + | - | - | - |
| bc | - | + | - | + | - | + | - | + | + | - | + | - | + | - | + | - |
| abc | - | - | - | - | - | - | - | - | + | + | + | + | + | + | + | + |
| d | - | + | + | - | + | - | - | + | - | + | + | - | + | - | - | + |
| ad | - | - | + | + | + | + | - | - | - | - | + | + | + | + | - | - |
| bd | - | + | - | + | + | - | + | - | - | + | - | + | + | + | + | - |
| abd | - | - | - | - | + | + | + | + | - | - | - | - | + | - | + | + |
| cd | - | + | + | - | - | + | + | - | - | + | + | - | - | - | + | - |
| acd | - | - | + | + | - | - | + | + | - | - | + | + | - | + | + | + |
| bcd | - | + | - | + | - | + | - | + | - | + | - | + | - | + | - | + |
| abcd | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - |

Tables C.1 Table Signs for Six Parameters Full Factorial Designs

(continued)

| | E F | A E F | B E F | A B E F | C E F | A C E F | B C E F | A B C E F | D E F | A D E F | B D E F | A B D E F | C D E F | A C D E F | B C D E F | A B C D E F |
|------|--------|-------------|-------------|------------------|-------------|------------------|------------------|-----------------------|-------------|------------------|------------------|-----------------------|------------------|-----------------------|-----------------------|----------------------------|
| (1) | + | - | - | + | - | + | + | - | - | + | + | - | + | - | - | + |
| a | + | + | - | - | - | - | + | + | - | - | + | + | + | + | - | - |
| b | + | - | + | - | - | - | - | + | - | + | - | + | + | + | - | + |
| ab | + | + | + | + | - | + | - | - | - | - | - | - | + | + | + | + |
| c | + | - | - | + | + | + | - | + | - | + | + | - | - | + | + | - |
| ac | + | + | - | - | + | + | - | - | - | - | + | - | + | - | + | + |
| bc | + | - | + | - | + | - | + | - | - | + | - | + | - | + | - | + |
| abc | + | + | + | + | + | + | + | + | - | - | - | - | - | - | - | - |
| d | + | - | - | + | - | + | + | - | + | - | - | + | - | + | + | - |
| ad | + | + | - | - | - | - | + | + | + | + | - | - | - | - | + | + |
| bd | + | - | + | - | - | - | - | + | + | - | + | - | - | + | - | + |
| abd | + | + | + | + | - | + | - | - | + | + | + | + | - | - | - | - |
| cd | + | - | - | + | + | + | - | + | + | - | - | + | + | - | - | + |
| acd | + | + | - | - | + | - | - | - | + | + | - | - | + | + | - | - |
| bcd | + | - | + | - | + | - | + | - | + | - | + | - | + | - | + | - |
| abcd | + | + | + | + | + | + | + | + | + | + | + | + | + | + | + | + |

Tables C.1 Table Signs for Six Parameters Full Factorial Designs

(continued)

| | A | B | A B | C | A C | B C | A B C | D | A D | B D | A B D | C D | A C D | B C D | A B C D |
|----|---|---|--------|---|--------|--------|-------------|---|--------|--------|-------------|--------|-------------|-------------|------------------|
| e | - | - | + | - | + | + | - | - | + | + | - | + | - | - | + |
| ae | + | - | - | - | - | + | + | - | - | + | + | + | + | - | - |
| be | - | + | - | - | - | - | + | - | + | - | + | + | + | + | - |

| | | | | | | | | | | | | | | |
|-------|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| abe | + | + | + | - | + | - | - | - | - | - | + | - | + | + |
| ce | - | - | + | + | + | - | + | - | + | + | - | - | + | - |
| ace | + | - | - | + | - | - | - | - | - | + | + | - | + | + |
| bce | - | + | - | + | - | + | - | - | + | - | + | - | + | + |
| abce | + | + | + | + | + | + | + | - | - | - | - | - | - | - |
| de | - | - | + | - | + | + | - | + | - | - | + | - | + | + |
| ade | + | - | - | - | - | + | + | + | + | - | - | - | - | + |
| bde | - | + | - | - | - | + | + | - | + | - | - | - | - | + |
| abde | + | + | + | - | + | - | - | + | + | + | + | - | + | - |
| cde | - | - | + | + | + | - | + | + | - | - | + | + | + | - |
| acde | + | - | - | + | - | - | - | + | + | - | - | + | - | - |
| bcde | - | + | - | + | - | + | - | + | - | + | - | + | - | - |
| abcde | + | + | + | + | + | + | + | + | + | + | + | + | + | + |

Tables C.1 Table Signs for Six Parameters Full Factorial Designs

(continued)

| | E | A E | B E | A B E | C E | A C E | B C E | A B C E | D E | A D E | B D E | A B D E | C D E | A C D E | B C D E | A B C D E |
|-------|---|-----|-----|-------|-----|-------|-------|---------|-----|-------|-------|---------|-------|---------|---------|-----------|
| e | + | - | - | + | - | + | + | - | - | + | + | - | + | - | - | + |
| ae | + | + | - | - | - | - | + | + | - | - | + | + | + | + | - | - |
| be | + | - | + | - | - | - | - | + | - | + | - | + | + | - | + | - |
| abe | + | + | + | + | - | + | - | - | - | - | - | - | + | + | + | + |
| ce | + | - | - | + | + | + | - | + | - | + | + | - | - | + | + | - |
| ace | + | + | - | - | + | - | - | - | - | + | + | - | - | - | + | + |
| bce | + | - | + | - | + | - | + | - | - | + | - | + | - | + | - | + |
| abce | + | + | + | + | + | + | + | + | - | - | - | - | - | - | - | - |
| de | + | - | - | + | - | + | + | - | + | - | - | + | - | + | + | - |
| ade | + | + | - | - | - | - | + | + | + | + | - | - | - | - | + | + |
| bde | + | - | + | - | - | - | - | + | + | - | + | - | - | + | - | + |
| abde | + | + | + | + | - | + | - | - | + | + | + | + | - | - | - | - |
| cde | + | - | - | + | + | + | - | + | + | - | - | + | + | - | - | + |
| acde | + | + | - | - | + | - | - | - | + | + | - | - | + | + | - | - |
| bcde | + | - | + | - | + | - | + | - | - | + | - | + | - | + | - | - |
| abcde | + | + | + | + | + | + | + | + | + | + | + | + | + | + | + | + |

Tables C.1 Table Signs for Six Parameters Full Factorial Designs

(continued)

| | F | A F | B F | A B F | C F | A C F | B C F | A B C F | D F | A D F | B D F | A B D F | C D F | A C D F | B C D F | A B C D F |
|-------|---|--------|--------|-------------|--------|-------------|-------------|------------------|--------|-------------|-------------|------------------|-------------|------------------|------------------|-----------------------|
| e | - | + | + | - | + | - | - | + | + | - | - | + | - | + | + | - |
| ae | - | - | + | + | + | + | - | - | + | - | + | - | - | - | - | + |
| be | - | + | - | + | + | - | + | - | + | - | + | - | - | - | - | + |
| abe | - | - | - | - | + | + | + | + | + | + | + | + | - | + | - | - |
| ce | - | + | + | - | - | + | + | - | + | - | - | + | + | + | - | + |
| ace | - | - | + | + | - | - | + | + | + | + | - | - | + | - | - | - |
| bce | - | + | - | + | - | + | - | + | + | - | + | - | + | - | + | - |
| abce | - | - | - | - | - | - | - | - | + | + | + | + | + | + | + | + |
| de | - | + | + | - | + | - | - | + | - | + | + | - | + | - | - | + |
| ade | - | - | + | + | + | + | - | - | - | - | + | + | + | + | - | - |
| bde | - | + | - | + | + | - | + | - | - | + | - | + | + | + | + | - |
| abde | - | - | - | - | + | + | + | + | - | - | - | - | + | - | + | + |
| cde | - | + | + | - | - | + | + | - | - | + | + | - | - | - | + | - |
| acde | - | - | + | + | - | - | + | + | - | - | + | + | - | + | + | + |
| bcde | - | + | - | + | - | + | - | + | - | + | - | + | - | + | - | + |
| abcde | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - |

Tables C.1 Table Signs for Six Parameters Full Factorial Designs

(continued)

| | E F | A E F | B E F | A B E F | C E F | A C E F | B C E F | A B C E F | D E F | A D E F | B D E F | A B D E F | C D E F | A C D E F | B C D E F | A B C D E F |
|----|--------|-------------|-------------|------------------|-------------|------------------|------------------|-----------------------|-------------|------------------|------------------|-----------------------|------------------|-----------------------|-----------------------|----------------------------|
| e | - | + | + | - | + | - | - | + | + | - | - | + | - | + | + | - |
| ae | - | - | + | + | + | + | - | - | + | + | - | - | - | - | - | + |

| | | | | | | | | | | | | | | | | |
|-------|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| be | - | + | - | + | + | + | + | - | + | - | + | - | - | + | - | + |
| abe | - | - | - | - | + | - | + | + | + | + | + | + | - | - | - | - |
| ce | - | + | + | - | - | - | + | - | + | - | - | + | + | - | - | + |
| ace | - | - | + | + | - | + | + | + | + | + | - | - | + | + | - | - |
| bce | - | + | - | + | - | + | - | + | + | - | + | - | + | - | + | - |
| abce | - | - | - | - | - | - | - | + | + | + | + | + | + | + | + | + |
| de | - | + | + | - | + | - | - | + | + | - | + | + | - | - | - | + |
| ade | - | - | + | + | + | + | - | - | - | - | + | + | + | + | - | - |
| bde | - | + | - | + | + | + | + | - | - | + | - | + | + | - | + | - |
| abde | - | - | - | - | + | - | + | + | - | - | - | - | + | + | + | + |
| cde | - | + | + | - | - | - | + | - | - | + | + | - | - | + | + | - |
| acde | - | - | + | + | - | + | + | + | - | - | + | + | - | - | + | + |
| bcde | - | + | - | + | - | + | - | + | - | + | - | + | - | + | - | + |
| abcde | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - |

Tables C.1 Table Signs for Six Parameters Full Factorial Designs

(continued)

| | A | B | A B | C | A C | B C | A B C | D | A D | B D | A B D | C D | A C D | B C D | A B C D |
|------|---|---|-----|---|-----|-----|-------|---|-----|-----|-------|-----|-------|-------|---------|
| f | - | - | + | - | + | + | - | - | + | + | - | + | - | - | + |
| af | + | - | - | - | - | + | + | - | - | + | + | + | + | - | - |
| bf | - | + | - | - | - | - | + | - | + | - | + | + | + | + | - |
| abf | + | + | + | - | + | - | - | - | - | - | - | + | - | + | + |
| cf | - | - | + | + | + | - | + | - | + | + | - | - | - | + | - |
| acf | + | - | - | + | - | - | - | - | - | + | + | - | + | + | + |
| bcf | - | + | - | + | - | + | - | - | + | - | + | - | + | - | + |
| abcf | + | + | + | + | + | + | + | - | - | - | - | - | - | - | - |
| df | - | - | + | - | + | + | - | + | - | - | + | - | + | + | - |
| adf | + | - | - | - | - | + | + | + | + | - | - | - | - | + | + |
| bdf | - | + | - | - | - | - | + | + | - | + | - | - | - | - | + |
| abdf | + | + | + | - | + | - | - | + | + | + | + | + | + | - | - |
| cdf | - | - | + | + | + | - | + | + | - | + | - | + | + | + | + |
| acd | + | - | - | + | - | - | - | + | + | - | - | + | + | - | - |
| bcd | - | + | - | + | - | + | - | + | - | + | - | + | - | + | - |
| abcd | + | + | + | + | + | + | + | + | + | + | + | + | + | + | + |

Tables C.1 Table Signs for Six Parameters Full Factorial Designs

(continued)

| | E | A E | B E | A B E | C E | A C E | B C E | A B C E | D E | A D E | B D E | A B D E | C D E | A C D E | B C D E | A B C D E |
|-------|---|-----|-----|-------|-----|-------|-------|---------|-----|-------|-------|---------|-------|---------|---------|-----------|
| f | - | + | + | - | + | - | - | + | + | - | - | + | - | + | + | - |
| af | - | - | + | + | + | + | - | - | + | + | - | - | - | - | + | + |
| bf | - | + | - | + | + | + | + | - | + | - | + | - | - | + | - | + |
| abf | - | - | - | - | + | - | + | + | + | + | + | + | - | - | - | - |
| cf | - | + | + | - | - | - | + | - | + | - | - | + | + | - | - | + |
| acf | - | - | + | + | - | + | + | + | + | + | - | - | + | + | - | - |
| bcf | - | + | - | + | - | + | - | + | + | - | + | - | + | - | + | - |
| abcf | - | - | - | - | - | - | - | + | + | + | + | + | + | + | + | + |
| df | - | + | + | - | + | - | - | + | - | + | + | - | + | - | - | + |
| adf | - | - | + | + | + | + | - | - | - | - | + | + | + | + | - | - |
| bdf | - | + | - | + | + | + | + | - | - | + | - | + | + | - | + | - |
| abdf | - | - | - | - | + | - | + | + | - | - | - | - | + | + | + | + |
| cdf | - | + | + | - | - | - | + | - | - | + | + | - | - | - | + | - |
| acdf | - | - | + | + | - | + | + | + | - | - | + | + | - | - | + | + |
| bcdf | - | + | - | + | - | + | - | + | - | + | - | + | - | + | - | + |
| abcdf | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - |

Tables C.1 Table Signs for Six Parameters Full Factorial Designs

(continued)

| | F | A F | B F | A B F | C F | A C F | B C F | A B C F | D F | A D F | B D F | A B D F | C D F | A C D F | B C D F | A B C D F |
|------|---|--------|--------|-------------|--------|-------------|-------------|------------------|--------|-------------|-------------|------------------|-------------|------------------|------------------|-----------------------|
| f | + | - | - | + | - | + | + | - | - | + | + | - | + | - | - | + |
| af | + | + | - | - | - | - | + | + | - | - | + | + | + | + | - | - |
| bf | + | - | + | - | - | + | - | + | - | + | - | + | + | + | + | - |
| abf | + | + | + | + | - | - | - | - | - | - | - | - | + | - | + | + |
| cf | + | - | - | + | + | - | - | + | - | + | + | - | - | - | + | - |
| acf | + | + | - | - | + | + | - | - | - | - | + | + | - | + | + | + |
| bcf | + | - | + | - | + | - | + | - | - | + | - | + | - | + | - | + |
| abcf | + | + | + | + | + | + | + | + | - | - | - | - | - | - | - | - |
| df | + | - | - | + | - | + | + | - | + | - | - | + | - | + | + | - |
| adf | + | + | - | - | - | - | + | + | + | + | - | - | - | - | + | + |
| bdf | + | - | + | - | - | + | - | + | + | - | + | - | - | - | - | + |
| abdf | + | + | + | + | - | - | - | - | + | + | + | + | - | + | - | - |
| cdf | + | - | - | + | + | - | - | + | - | - | + | + | + | + | - | + |
| acdf | + | + | - | - | + | + | - | - | + | + | - | - | + | - | - | - |
| bcd | + | - | + | - | + | - | + | - | + | - | + | - | + | - | + | - |
| abcd | + | + | + | + | + | + | + | + | + | + | + | + | + | + | + | + |

Tables C.1 Table Signs for Six Parameters Full Factorial Designs

(continued)

| | E F | A E F | B E F | A B E F | C E F | A C E F | B C E F | A B C E F | D E F | A D E F | B D E F | A B D E F | C D E F | A C D E F | B C D E F | A B C D E F |
|-------|--------|-------------|-------------|------------------|-------------|------------------|------------------|-----------------------|-------------|------------------|------------------|-----------------------|------------------|-----------------------|-----------------------|----------------------------|
| f | - | + | + | - | + | - | - | + | + | - | - | + | - | + | + | - |
| af | - | - | + | + | + | + | - | + | + | - | - | - | - | - | + | + |
| bf | - | + | - | + | + | + | + | - | + | - | + | - | - | + | - | + |
| abf | - | - | - | - | + | - | + | + | + | + | + | + | - | - | - | - |
| cf | - | + | + | - | - | - | + | - | + | - | - | + | + | - | - | + |
| acf | - | - | + | + | - | + | + | + | + | + | - | - | + | + | - | - |
| bcf | - | + | - | + | - | + | - | + | + | - | + | - | + | - | + | - |
| abcf | - | - | - | - | - | - | - | - | + | + | + | + | + | + | + | + |
| df | - | + | + | - | + | - | - | + | - | + | + | - | + | - | - | + |
| adf | - | - | + | + | + | + | - | - | - | - | + | + | + | + | - | - |
| bdf | - | + | - | + | + | + | + | - | + | - | + | + | + | - | + | - |
| abdf | - | - | - | - | + | - | + | + | - | - | - | - | + | + | + | + |
| cdf | - | + | + | - | - | - | + | - | - | + | + | - | - | + | + | - |
| acdf | - | - | + | + | - | + | + | + | - | - | + | + | - | - | + | + |
| bcdf | - | + | - | + | - | + | - | + | - | + | - | + | - | + | - | + |
| abcdf | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - |

Tables C.1 Table Signs for Six Parameters Full Factorial Designs

(continued)

| | A | B | A B | C | A C | B C | A B C | D | A D | B D | A B D | C D | A C D | B C D | A B C D | A B C D E F |
|--------|---|---|--------|---|--------|--------|-------------|---|--------|--------|-------------|--------|-------------|-------------|------------------|----------------------------|
| ef | - | - | + | - | + | + | - | - | + | + | - | + | - | - | + | - |
| aef | + | - | - | - | - | + | + | - | - | + | + | + | + | - | - | + |
| bef | - | + | - | - | - | + | + | - | + | - | + | + | + | + | + | - |
| abef | + | + | + | - | + | - | - | - | - | - | + | + | - | + | + | - |
| cef | - | - | + | + | + | - | + | - | + | + | - | - | - | + | - | + |
| acef | + | - | - | + | - | - | - | - | + | + | - | + | + | + | + | - |
| bcef | - | + | - | + | - | + | - | - | + | - | + | - | + | - | + | - |
| abcef | + | + | + | + | + | + | + | - | - | - | - | - | - | - | - | + |
| def | - | - | + | - | + | + | - | + | - | - | + | - | + | + | - | + |
| adef | + | - | - | - | - | + | + | + | + | - | - | - | - | + | + | - |
| bdef | - | + | - | - | - | - | + | + | - | + | - | - | - | - | + | - |
| abdef | + | + | + | - | + | - | - | + | + | + | + | + | + | - | - | + |
| cdef | - | - | + | + | + | - | + | + | - | - | + | + | + | - | + | - |
| acdef | + | - | - | + | - | - | - | + | + | - | - | + | - | - | - | + |
| bcdef | - | + | - | + | - | + | - | + | - | + | - | + | - | + | - | + |
| abcdef | + | + | + | + | + | + | + | + | + | + | + | + | + | + | + | - |

Tables C.1 Table Signs for Six Parameters Full Factorial Designs

(continued)

| | E | A E | B E | A B E | C E | A C E | B C E | A B C E | D E | A D E | B D E | A B D E | C D E | A C D E | B C D E | A B C D E |
|------|---|--------|--------|-------------|--------|-------------|-------------|------------------|--------|-------------|-------------|------------------|-------------|------------------|------------------|-----------------------|
| ef | + | - | - | + | - | + | + | - | - | + | + | - | + | - | - | + |
| aef | + | + | - | - | - | + | + | + | - | - | + | + | + | + | - | - |
| bef | + | - | + | - | - | - | - | + | - | + | - | + | + | + | - | - |
| abef | + | + | + | + | - | + | - | - | - | - | - | - | + | + | + | + |

| | | | | | | | | | | | | | | | | |
|--------|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| cef | + | - | - | + | + | + | - | + | - | + | + | - | - | + | + | - |
| acef | + | + | - | - | + | - | - | - | - | - | + | + | - | - | + | + |
| bcef | + | - | + | - | + | - | + | - | - | + | - | + | - | + | - | + |
| abcef | + | + | + | + | + | + | + | + | - | - | - | - | - | - | - | - |
| def | + | - | - | + | - | + | + | - | + | - | - | + | - | + | + | - |
| adeff | + | + | - | - | - | - | + | + | + | + | - | - | - | - | + | + |
| bdef | + | - | + | - | - | - | - | + | + | - | + | - | - | + | - | + |
| abdef | + | + | + | + | - | + | - | - | + | + | + | + | - | - | - | - |
| cdef | + | - | - | + | + | + | - | + | + | - | - | + | + | - | - | + |
| acdef | + | + | - | - | + | - | - | - | + | + | - | - | + | + | - | - |
| bcdef | + | - | + | - | + | - | + | - | + | - | + | - | + | - | + | - |
| abcdef | + | + | + | + | + | + | + | + | + | + | + | + | + | + | + | + |

Tables C.1 Table Signs for Six Parameters Full Factorial Designs

(continued)

| | F | A F | B F | A B F | C F | A C F | B C F | A B C F | D F | A D F | B D F | A B D F | C D F | A C D F | B C D F | A B C D F |
|--------|---|--------|--------|-------------|--------|-------------|-------------|------------------|--------|-------------|-------------|------------------|-------------|------------------|------------------|-----------------------|
| ef | + | - | - | + | - | + | + | - | - | + | + | - | + | - | - | + |
| aef | + | + | - | - | - | - | + | + | - | - | + | + | + | + | - | - |
| bef | + | - | + | - | - | + | - | + | - | + | - | + | + | + | + | - |
| abef | + | + | + | + | - | - | - | - | - | - | - | - | + | - | + | + |
| cef | + | - | - | + | + | - | - | + | - | + | + | - | - | - | + | - |
| acef | + | + | - | - | + | + | - | - | - | - | + | + | - | + | + | + |
| bcef | + | - | + | - | + | - | + | - | - | + | - | + | - | + | - | + |
| abcef | + | + | + | + | + | + | + | + | - | - | - | - | - | - | - | - |
| def | + | - | - | + | - | + | + | - | + | - | - | + | - | + | + | - |
| adeff | + | + | - | - | - | - | + | + | + | + | - | - | - | - | + | + |
| bdef | + | - | + | - | - | + | - | + | + | - | + | - | - | - | - | + |
| abdef | + | + | + | + | - | - | - | - | + | + | + | + | - | + | - | - |
| cdef | + | - | - | + | + | - | - | + | + | - | - | + | + | + | - | + |
| acdef | + | + | - | - | + | + | - | + | + | + | - | + | + | - | - | - |
| bcdef | + | - | + | - | + | - | + | - | + | - | + | - | + | - | + | - |
| abcdef | + | + | + | + | + | + | + | + | + | + | + | + | + | + | + | + |

Tables C.1 Table Signs for Six Parameters Full Factorial Designs

(continued)

| | E F | A E F | B E F | A B E F | C E F | A C E F | B C E F | A B C E F | D E F | A D E F | B D E F | A B D E F | C D E F | A C D E F | B C D E F | A B C D E F |
|--------|--------|-------------|-------------|------------------|-------------|------------------|------------------|-----------------------|-------------|------------------|------------------|-----------------------|------------------|-----------------------|-----------------------|----------------------------|
| ef | + | - | - | + | - | + | + | - | - | + | + | - | + | - | - | + |
| aef | + | + | - | - | - | - | + | + | - | - | + | + | + | + | - | - |
| bef | + | - | + | - | - | - | - | + | - | + | - | + | + | - | + | - |
| abef | + | + | + | + | - | + | - | - | - | - | - | - | + | + | + | + |
| cef | + | - | - | + | + | + | - | + | - | + | + | - | - | + | + | - |
| acef | + | + | - | - | + | - | - | - | - | + | + | - | - | + | + | + |
| bcef | + | - | + | - | + | - | + | - | - | + | - | + | - | + | - | + |
| abcef | + | + | + | + | + | + | + | + | - | - | - | - | - | - | - | - |
| def | + | - | - | + | - | + | + | - | + | - | - | + | - | + | + | - |
| adef | + | + | - | - | - | - | + | + | + | + | - | - | - | - | + | + |
| bdef | + | - | + | - | - | - | - | + | - | + | - | + | - | + | - | + |
| abdef | + | + | + | + | - | + | - | - | + | + | + | + | - | - | - | - |
| cdef | + | - | - | + | + | + | - | + | + | - | - | + | + | - | - | + |
| acdef | + | + | - | - | + | - | - | - | + | + | - | - | + | + | - | - |
| bcdef | + | - | + | - | + | - | + | - | + | - | + | - | + | - | + | - |
| abcdef | + | + | + | + | + | + | + | + | + | + | + | + | + | + | + | + |

Table C.2 Table Signs Six Parameters One-Half Fractional Factorial

Designs

| | A | B | C | D | E | F | AB | AC | AD | AE | AF | BC | BD | BE | BF | CD |
|--------|---|---|---|---|---|---|----|----|----|----|----|----|----|----|----|----|
| (1) | - | - | - | - | - | - | + | + | + | + | + | + | + | + | + | + |
| af | + | - | - | - | - | + | - | - | - | - | - | + | + | + | + | + |
| bf | - | + | - | - | - | + | - | - | + | + | + | - | - | - | - | + |
| ab | + | + | - | - | - | - | + | + | - | - | - | - | - | - | - | + |
| cf | - | - | + | - | - | + | + | + | + | + | + | - | + | + | + | - |
| ac | + | - | + | - | - | - | - | - | - | - | - | - | + | + | + | - |
| bc | - | + | + | - | - | - | - | - | + | + | + | + | - | - | - | - |
| abcf | + | + | + | - | - | + | + | + | - | - | - | + | - | - | - | - |
| df | - | - | - | + | - | + | + | + | - | + | + | + | - | + | + | - |
| ad | + | - | - | + | - | - | - | - | + | - | - | + | - | + | + | - |
| bd | - | + | - | + | - | - | - | - | - | + | + | - | + | - | - | - |
| abdf | + | + | - | + | - | + | + | + | + | - | - | - | + | - | - | - |
| cd | - | - | + | + | - | - | + | + | - | + | + | - | - | + | + | + |
| acdf | + | - | + | + | - | + | - | - | + | - | - | - | - | + | + | + |
| bcdf | - | + | + | + | - | + | - | - | - | + | + | + | + | - | - | + |
| abcd | + | + | + | + | - | - | + | + | + | - | - | + | + | - | - | + |
| ef | - | - | - | - | + | + | + | + | + | - | + | + | + | - | + | + |
| ae | + | - | - | - | + | - | - | - | - | + | - | + | + | - | + | + |
| be | - | + | - | - | + | - | - | - | + | - | + | - | - | + | - | + |
| abef | + | + | - | - | + | + | + | + | - | + | - | - | - | + | - | + |
| ce | - | - | + | - | + | - | + | + | + | - | + | - | + | - | + | - |
| acef | + | - | + | - | + | + | - | - | - | + | - | - | + | - | + | - |
| bcef | - | + | + | - | + | + | - | - | + | - | + | + | - | + | - | - |
| abce | + | + | + | - | + | - | + | + | - | + | - | + | - | + | - | - |
| de | - | - | - | + | - | + | + | + | - | - | + | + | - | - | + | - |
| adef | + | - | - | + | + | + | - | - | + | + | - | + | - | - | + | - |
| bdef | - | + | - | + | + | + | - | - | - | - | + | - | + | + | - | - |
| abde | + | + | - | + | + | - | + | + | + | + | - | - | + | + | - | - |
| cdef | - | - | + | + | + | + | + | + | - | - | + | - | - | - | + | + |
| acde | + | - | + | + | + | - | - | - | + | + | - | - | - | - | + | + |
| bcde | - | + | + | + | + | - | - | - | - | - | + | + | + | + | - | + |
| abcdef | + | + | + | + | + | + | + | + | + | + | - | + | + | + | - | + |

Table C.2 Table Signs Six Parameters One-Half Fractional Factorial

Designs (continued)

| | CE | CF | DE | DF | EF | ABC | ABD | ABE | ABF | ACD | ACE | ACF | ADE | ADF | AEF |
|-------|----|----|----|----|----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|
| (1) | + | + | + | + | + | - | - | - | - | - | - | - | - | - | - |
| af | + | + | + | + | + | + | + | + | + | + | + | + | + | + | + |
| bf | + | + | + | + | + | + | + | + | + | + | + | - | - | - | - |
| ab | + | + | + | + | + | - | - | - | - | - | - | + | + | + | + |
| cf | - | - | + | + | + | + | - | - | - | - | - | + | - | - | - |
| ac | - | - | + | + | + | - | + | + | + | + | + | - | + | + | + |
| bc | - | - | + | + | + | - | + | + | + | + | + | + | - | - | - |
| abcf | - | - | + | + | + | + | - | - | - | - | - | - | + | + | + |
| df | + | + | - | - | + | - | + | - | - | + | - | - | + | + | - |
| ad | + | + | - | - | + | + | - | + | + | - | + | + | - | - | + |
| bd | + | + | - | - | + | + | - | + | + | - | + | - | + | + | - |
| abdf | + | + | - | - | + | - | + | - | - | + | - | + | - | - | + |
| cd | - | - | - | - | + | + | + | - | - | + | - | + | + | + | - |
| acdf | - | - | - | - | + | - | - | + | + | - | + | - | - | - | + |
| bcd | - | - | - | - | + | - | - | + | + | - | + | + | + | + | - |
| abcd | - | - | - | - | + | + | + | - | - | + | - | - | - | - | + |
| ef | - | + | - | + | - | - | - | + | - | - | + | - | + | - | + |
| ae | - | + | - | + | - | + | + | - | + | + | - | + | - | + | - |
| be | - | + | - | + | - | + | + | - | + | + | - | - | + | - | + |
| abef | - | + | - | + | - | - | - | + | - | - | + | + | - | + | - |
| ce | + | - | - | + | - | + | - | + | - | - | + | + | + | - | + |
| acef | + | - | - | + | - | - | + | - | + | + | - | - | - | + | - |
| bcef | + | - | - | + | - | - | + | - | + | + | - | + | + | - | + |
| abce | + | - | - | + | - | + | - | + | - | - | + | - | + | + | - |
| de | - | + | + | - | - | - | + | + | - | + | + | - | - | + | + |
| adef | - | + | + | - | - | + | - | - | + | - | - | + | + | - | - |
| bdef | - | + | + | - | - | + | - | - | + | - | - | - | - | + | + |
| abde | - | + | + | - | - | - | + | + | - | + | + | + | + | - | - |
| cdef | + | - | + | - | - | + | + | + | - | + | + | + | - | + | + |
| acde | + | - | + | - | - | - | - | - | + | - | - | - | + | - | - |
| bcde | + | - | + | - | - | - | - | - | + | - | - | + | - | + | + |
| abcde | + | - | + | - | - | + | + | + | - | + | + | - | + | - | - |
| f | | | | | | | | | | | | | | | |

APPENDIX D

Additional Results

Table D. 1 The Effect Estimation based on the response of R^2 calculated using FF and OHF.

| Par/Interac. | Effects | |
|--------------|-----------|-----------|
| | FF | OHF |
| A | -0.00125 | -0.00127 |
| B | -0.00398 | -0.00398 |
| AB | -0.0002 | -0.00027 |
| C | -0.03145 | -0.03145 |
| AC | -0.0002 | -0.00027 |
| BC | 0.004498 | 0.004498 |
| ABC | -9.30E-06 | 0.000892 |
| D | -0.001 | -0.001 |
| AD | -0.00169 | -0.00163 |
| BD | 0.006497 | 0.006496 |
| ABD | 4.98E-05 | -9.40E-05 |
| CD | -0.04533 | -0.04533 |
| ACD | 4.98E-05 | -9.40E-05 |
| BCD | 0.000428 | =AEF |
| ABCD | -1.10E-06 | =EF |
| E | -0.01366 | -0.01366 |
| AE | 0.000332 | 0.000309 |
| BE | 0.005262 | 0.005262 |
| ABE | 0.000198 | 0.000129 |
| CE | 0.003363 | 0.003363 |
| ACE | 0.000198 | 0.000129 |
| BCE | -0.00038 | =ADF |
| ABCE | 9.16E-06 | =DF |
| DE | -0.00757 | -0.00757 |
| ADE | -0.00023 | -0.00016 |
| BDE | -0.0025 | =ACF |
| ABDE | -5.30E-05 | =CF |
| CDE | 0.001219 | =ABF |
| ACDE | -1.90E-05 | =BF |
| BCDE | 0.000228 | =AF |
| ABCDE | 9.06E-07 | =F |
| F | 0.001332 | 0.001333 |
| AF | -2.80E-07 | 0.001273 |
| BF | -0.00068 | 0.003975 |
| ABF | -3.10E-08 | 0.000271 |
| CF | -0.00014 | 0.03145 |
| ACF | -9.40E-08 | 0.003985 |
| BCF | 6.78E-05 | =ADE |
| ABCF | -9.40E-08 | =DE |
| DF | 0.000901 | 0.001003 |
| ADF | -1.60E-07 | 0.001627 |
| BDF | 0.000226 | =ACE |

| | | |
|--------|-----------|----------|
| ABDF | -3.10E-08 | =CE |
| CDF | -6.90E-05 | =ABE |
| ACDF | -3.10E-08 | =BE |
| BCDF | -2.30E-05 | =AE |
| ABCDF | 3.13E-08 | =E |
| EF | 0.001332 | 0.013658 |
| AEF | -2.80E-07 | -0.00031 |
| BEF | -0.00068 | =ACD |
| ABEF | -3.10E-08 | =CD |
| CEF | -0.00014 | =ABD |
| ACEF | -3.10E-08 | =BD |
| BCEF | 6.78E-05 | =AD |
| ABCEF | -9.40E-08 | =D |
| DEF | 0.000901 | =ABC |
| ADEF | -1.60E-07 | =BC |
| BDEF | 0.000226 | =AC |
| ABDEF | -3.10E-08 | =C |
| CDEF | -6.90E-05 | =AB |
| ACDEF | -9.40E-08 | =B |
| BCDEF | -2.30E-05 | =A |
| ABCDEF | 3.13E-08 | =I |

Table D.2 The Effect Estimation based on the response of Dv calculated using FF and OHF.

| Par/Interac. | Effects | |
|--------------|-----------|-----------|
| | FF | OHF |
| A | -0.0003 | -0.00023 |
| B | 0.013224 | 0.013225 |
| AB | -5.90E-05 | 2.49E-04 |
| C | 0.128277 | 0.128277 |
| AC | -5.90E-05 | 2.49E-04 |
| BC | 6.95E-03 | 6.95E-03 |
| ABC | -5.90E-05 | 8.27E-04 |
| D | 0.255746 | 0.255746 |
| AD | -2.30E-03 | -2.28E-03 |
| BD | 1.41E-02 | 1.41E-02 |
| ABD | 5.91E-05 | 5.60E-04 |
| CD | 0.43193 | 0.43193 |
| ACD | 5.91E-05 | 5.60E-04 |
| BCD | 2.42E-03 | AEF |
| ABCD | 5.91E-05 | EF |
| E | 0.003659 | 0.003659 |
| AE | 0.000269 | 0.000338 |
| BE | -2.99E-03 | -2.99E-03 |
| ABE | 5.90E-05 | 3.67E-04 |
| CE | 2.90E-03 | 2.90E-03 |

| | | |
|--------|-----------|-----------|
| ACE | 5.90E-05 | 3.67E-04 |
| BCE | -1.14E-03 | ADF |
| ABCE | 5.92E-05 | DF |
| DE | 4.47E-04 | 4.47E-04 |
| ADE | 4.86E-04 | 5.05E-04 |
| BDE | -1.77E-03 | ACF |
| ABDE | -5.90E-05 | CF |
| CDE | -3.40E-04 | ABF |
| ACDE | 2.19E-04 | BF |
| BCDE | 1.43E-05 | AF |
| ABCDE | -5.90E-05 | F |
| F | 0.000797 | 0.000738 |
| AF | 3.12E-08 | 0.000227 |
| BF | 2.96E-04 | -0.01322 |
| ABF | 3.13E-08 | -2.50E-04 |
| CF | 5.00E-04 | -0.12828 |
| ACF | 3.12E-08 | 7.96E-04 |
| BCF | 1.92E-05 | ADE |
| ABCF | 3.13E-08 | DE |
| DF | 8.86E-04 | -0.25575 |
| ADF | -3.10E-08 | 2.29E-03 |
| BDF | 2.39E-04 | ACE |
| ABDF | -1.60E-07 | CE |
| CDF | 3.08E-04 | ABE |
| ACDF | -1.60E-07 | BE |
| BCDF | 6.97E-05 | AE |
| ABCDF | -3.10E-08 | E |
| EF | 0.000797 | -0.00366 |
| AEF | 3.12E-08 | -0.00034 |
| BEF | 2.96E-04 | ACD |
| ABEF | 3.13E-08 | CD |
| CEF | 5.00E-04 | ABD |
| ACEF | 3.13E-08 | BD |
| BCEF | 1.92E-05 | AD |
| ABCEF | 3.13E-08 | D |
| DEF | 8.86E-04 | ABC |
| ADEF | -3.10E-08 | BC |
| BDEF | 2.39E-04 | AC |
| ABDEF | -1.60E-07 | C |
| CDEF | 3.08E-04 | AB |
| ACDEF | 9.37E-08 | B |
| BCDEF | 6.97E-05 | A |
| ABCDEF | -3.10E-08 | I |

Table D.3 The ANOVA Table of The Polynomial model developed using CCD based on 1-year Calibration Data

| Factor | Coefficient Estimate | DF | Standard Error | t for H0 Coeff=0 | Prob > t |
|-----------|----------------------|----|----------------|------------------|-----------|
| Intercept | 160.166 | 1 | 6.43138 | | |
| B-B | 12.2031 | 1 | 4.3143 | 2.82852 | 0.0060 |
| C-C | -1.20E+00 | 1 | 4.31E+00 | -0.27811 | 0.7817 |
| D-D | 0.46244 | 1 | 4.3143 | 0.107188 | 0.9149 |
| E-E | 2.72E+01 | 1 | 4.31E+00 | 6.31478 | < 0.0001 |
| C2 | 2.34E+01 | 1 | 3.57271 | 6.55165 | < 0.0001 |
| D2 | 2.73E+01 | 1 | 3.57271 | 7.63457 | < 0.0001 |
| BD | -8.70047 | 1 | 4.82353 | -1.80375 | 0.0753 |
| BE | -1.36E+01 | 1 | 4.82353 | -2.82927 | 0.0060 |
| CD | 1.42E+01 | 1 | 4.82E+00 | 2.95043 | 0.0042 |
| CE | -9.41E+00 | 1 | 4.82E+00 | -1.95117 | 0.0548 |
| DE | 13.944 | 1 | 4.82353 | 2.89083 | 0.0050 |

- $/E/ = 27.919$
- $R^2 = 0.9978$
- $Dv = 0.2831$

Table D.4 The ANOVA Table of The Polynomial model developed using CCD based on 2-years Calibration Data

| Factor | Coefficient Estimate | DF | Standard Error | t for H0 Coeff=0 | Prob > t |
|-----------|----------------------|----|----------------|------------------|-----------|
| Intercept | 239.278 | 1 | 12.8911 | | |
| C-C | 20.48 | 1 | 8.64759 | 2.36828 | 0.0203 |
| D-D | 1.72E+01 | 1 | 8.65E+00 | 1.98772 | 0.0503 |
| E-E | 27.1331 | 1 | 8.64759 | 3.13765 | 0.0024 |
| C2 | 6.95E+01 | 1 | 7.16E+00 | 9.70568 | < 0.0001 |
| D2 | 7.82E+01 | 1 | 7.16115 | 10.9233 | < 0.0001 |
| CD | 5.36E+01 | 1 | 9.6683 | 5.54524 | < 0.0001 |

- $/E/ = 91.1368$
- $R^2 = 0.9976$
- $Dv = 0.2386$

Table D.5 The ANOVA Table of The Polynomial model developed using CCD based on 3-years Calibration Data

| Factor | Coefficient Estimate | DF | Standard Error | t for H0 Coeff=0 | Prob > t |
|-----------|----------------------|----|----------------|------------------|-----------|
| Intercept | 350.136 | 1 | 13.8618 | | |
| C-C | 45.2559 | 1 | 9.29877 | 4.86687 | < 0.0001 |
| D-D | 7.69E+00 | 1 | 9.30E+00 | 0.827367 | 0.4105 |
| E-E | 28.3854 | 1 | 9.29877 | 3.05259 | 0.0031 |
| C2 | 1.27E+02 | 1 | 7.70E+00 | 16.4541 | < 0.0001 |
| D2 | 1.07E+02 | 1 | 7.70039 | 13.8638 | < 0.0001 |
| CD | 9.63E+01 | 1 | 10.3963 | 9.26517 | < 0.0001 |

- $/E/ = 107.2714$
- $R^2 = 0.9979$
- $Dv = 0.3161$

Table D.6 The ANOVA Table of The Polynomial model developed using BBD based on 1-year Calibration Data

| Factor | Coefficient Estimate | DF | Standard Error | t for H0 Coeff=0 | Prob > t |
|-----------|----------------------|----|----------------|------------------|-----------|
| Intercept | 175.502 | 1 | 4.8927 | | |
| B-B | 12.6466 | 1 | 3.58109 | 3.53149 | 0.0011 |
| C-C | 2.43E+00 | 1 | 3.58E+00 | 0.678176 | 0.5017 |
| D-D | -17.3118 | 1 | 3.58109 | -4.83424 | < 0.0001 |
| E-E | 3.71E+01 | 1 | 3.58E+00 | 10.3721 | < 0.0001 |
| F-F | -2.23E+01 | 1 | 3.58109 | -6.23215 | < 0.0001 |
| B2 | 1.25E+01 | 1 | 5.31161 | 2.36027 | 0.0234 |
| C2 | 37.3107 | 1 | 5.31161 | 7.02437 | < 0.0001 |
| E2 | -2.18E+01 | 1 | 5.31161 | -4.09813 | 0.0002 |
| F2 | -1.59E+01 | 1 | 5.31E+00 | -2.9987 | 0.0047 |
| BE | -1.53E+01 | 1 | 4.39E+00 | -3.47911 | 0.0013 |
| CD | 14.7394 | 1 | 6.20263 | 2.37631 | 0.0225 |
| CF | 1.01E+01 | 1 | 4.39E+00 | 2.29866 | 0.0270 |
| DE | 1.61E+01 | 1 | 6.20263 | 2.60191 | 0.0130 |
| DF | -1.45E+01 | 1 | 6.20263 | -2.33365 | 0.0249 |

- $/E/ = 40.9926$
- $R^2 = 0.9958$
- $Dv = 0.4658$

Table D.7 The ANOVA Table of The Polynomial model developed using BBD based on 2-year Calibration Data

| Factor | Coefficient Estimate | DF | Standard Error | t for H0 Coeff=0 | Prob > t |
|-----------|----------------------|----|----------------|------------------|-----------|
| Intercept | 249.893 | 1 | 7.65969 | | |
| B-B | 12.2303 | 1 | 4.25664 | 2.87323 | 0.0066 |
| C-C | 1.82E+01 | 1 | 4.26E+00 | 4.27116 | 0.0001 |
| D-D | -30.1225 | 1 | 4.25664 | -7.0766 | < 0.0001 |
| E-E | 3.70E+01 | 1 | 4.26E+00 | 8.70336 | < 0.0001 |
| F-F | -2.22E+01 | 1 | 4.25664 | -5.20872 | < 0.0001 |
| B2 | 1.24E+01 | 1 | 6.43543 | 1.92886 | 0.0612 |
| C2 | 123.546 | 1 | 6.43543 | 19.1978 | < 0.0001 |
| D2 | 2.62E+01 | 1 | 6.23108 | 4.19878 | 0.0002 |
| E2 | -2.12E+01 | 1 | 6.44E+00 | -3.29834 | 0.0021 |
| F2 | -2.07E+01 | 1 | 6.44E+00 | -3.21175 | 0.0027 |
| BE | -15.2591 | 1 | 5.21329 | -2.92697 | 0.0058 |
| CD | 5.45E+01 | 1 | 7.37E+00 | 7.3961 | < 0.0001 |
| CF | 1.06E+01 | 1 | 5.21329 | 2.02511 | 0.0499 |
| DE | 1.59E+01 | 1 | 7.37271 | 2.15121 | 0.0379 |
| DF | -14.3824 | 1 | 7.37271 | -1.95076 | 0.0585 |

- $/E/ = 93.5997$
- $R^2 = 0.9975$
- $Dv = 0.2529$

Table D.8 The ANOVA Table of The Polynomial model developed using BBD based on 3-year Calibration Data

| Factor | Coefficient Estimate | DF | Standard Error | t for H0 Coeff=0 | Prob > t |
|-----------|----------------------|----|----------------|------------------|-----------|
| Intercept | 317.385 | 1 | 8.54514 | | |
| A-A | 4.73092 | 1 | 6.2544 | 0.756413 | 0.4537 |
| B-B | 1.23E+01 | 1 | 6.25E+00 | 1.95971 | 0.0569 |
| C-C | 42.8414 | 1 | 6.2544 | 6.8498 | < 0.0001 |
| D-D | -5.80E+01 | 1 | 6.25E+00 | -9.26697 | < 0.0001 |
| E-E | 3.84E+01 | 1 | 6.2544 | 6.1426 | < 0.0001 |
| F-F | -2.22E+01 | 1 | 6.2544 | -3.54652 | 0.0010 |
| A2 | 20.4186 | 1 | 9.27678 | 2.20105 | 0.0334 |
| C2 | 2.32E+02 | 1 | 9.27678 | 24.9645 | < 0.0001 |
| D2 | 6.86E+01 | 1 | 9.28E+00 | 7.39492 | < 0.0001 |
| F2 | -2.90E+01 | 1 | 9.28E+00 | -3.12408 | 0.0033 |
| BE | -15.2595 | 1 | 7.66005 | -1.99208 | 0.0530 |
| CD | 9.81E+01 | 1 | 1.08E+01 | 9.05268 | < 0.0001 |

- $/E/ = 107.9525$
- $R^2 = 0.9978$
- $Dv = 0.3721$

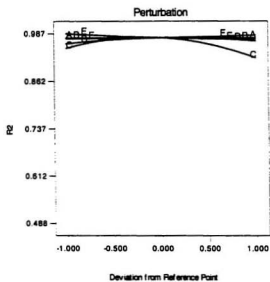


Fig. D.1 The Perturbation Plot of the Mock Model-Parameters Based on R^2

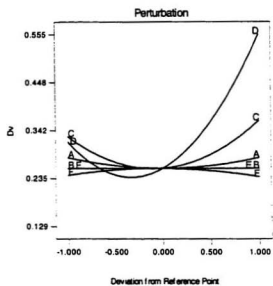


Fig. D. 3 The Perturbation Plot of the Mock Model-Parameters Based on

Dv

Appendix E

Input Data

Table E. 1 The Data of Rainfall, Evapotranspiration and Runoff

| Year | Month | Rainfall | Evapo-transpiration | Runoff |
|------|-------|----------|---------------------|--------|
| 1973 | Jan | 170 | 102.3 | 139 |
| 1973 | Feb | 165 | 98 | 51 |
| 1973 | Mar | 110 | 108.5 | 45 |
| 1973 | Apr | 265 | 102 | 76 |
| 1973 | May | 378 | 102.3 | 198 |
| 1973 | Jun | 350 | 90 | 203 |
| 1973 | Jul | 191 | 89.9 | 123 |
| 1973 | Aug | 198 | 105.4 | 116 |
| 1973 | Sep | 230 | 114 | 116 |
| 1973 | Oct | 220 | 127.1 | 105 |
| 1973 | Nov | 240 | 117 | 123 |
| 1973 | Dec | 108 | 105.4 | 49 |
| 1974 | Jan | 118 | 102.3 | 111 |
| 1974 | Feb | 77 | 98 | 40 |
| 1974 | Mar | 310 | 108.5 | 141 |
| 1974 | Apr | 275 | 102 | 140 |
| 1974 | May | 305 | 102.3 | 165 |
| 1974 | Jun | 442 | 90 | 263 |
| 1974 | Jul | 390 | 89.9 | 247 |
| 1974 | Aug | 350 | 105.4 | 241 |
| 1974 | Sep | 420 | 114 | 281 |
| 1974 | Oct | 296 | 127.1 | 218 |
| 1974 | Nov | 235 | 117 | 151 |
| 1974 | Dec | 25 | 105.4 | 90 |
| 1975 | Jan | 48 | 102.3 | 64 |
| 1975 | Feb | 67 | 98 | 51 |
| 1975 | Mar | 13 | 108.5 | 33 |
| 1975 | Apr | 150 | 102 | 40 |
| 1975 | May | 250 | 102.3 | 89 |
| 1975 | Jun | 150 | 90 | 56 |
| 1975 | Jul | 275 | 89.9 | 122 |
| 1975 | Aug | 577 | 105.4 | 312 |
| 1975 | Sep | 248 | 114 | 172 |
| 1975 | Oct | 165 | 127.1 | 101 |
| 1975 | Nov | 98 | 117 | 64 |
| 1975 | Dec | 68 | 105.4 | 55 |
| 1976 | Jan | 80 | 102.3 | 35 |
| 1976 | Feb | 77 | 98 | 34 |
| 1976 | Mar | 167 | 108.5 | 83 |
| 1976 | Apr | 480 | 102 | 262 |
| 1976 | May | 568 | 102.3 | 342 |

| | | | | |
|------|-----|-----|-------|-----|
| 1976 | Jun | 370 | 90 | 252 |
| 1976 | Jul | 335 | 89.9 | 234 |
| 1976 | Aug | 115 | 105.4 | 96 |
| 1976 | Sep | 130 | 114 | 96 |
| 1976 | Oct | 78 | 127.1 | 57 |
| 1976 | Nov | 95 | 117 | 54 |
| 1976 | Dec | 45 | 105.4 | 39 |
| 1977 | Jan | 10 | 102.3 | 29 |
| 1977 | Feb | 12 | 98 | 19 |
| 1977 | Mar | 20 | 108.5 | 4 |
| 1977 | Apr | 38 | 102 | 15 |
| 1977 | May | 67 | 102.3 | 25 |
| 1977 | Jun | 305 | 90 | 67 |
| 1977 | Jul | 308 | 89.9 | 141 |
| 1977 | Aug | 227 | 105.4 | 113 |
| 1977 | Sep | 280 | 114 | 144 |
| 1977 | Oct | 150 | 127.1 | 85 |
| 1977 | Nov | 310 | 117 | 184 |
| 1977 | Dec | 348 | 105.4 | 197 |
| 1978 | Jan | 41 | 102.3 | 68 |
| 1978 | Feb | 145 | 98 | 59 |
| 1978 | Mar | 175 | 108.5 | 48 |
| 1978 | Apr | 508 | 102 | 279 |
| 1978 | May | 406 | 102.3 | 301 |
| 1978 | Jun | 245 | 90 | 173 |
| 1978 | Jul | 368 | 89.9 | 244 |
| 1978 | Aug | 530 | 105.4 | 342 |
| 1978 | Sep | 585 | 114 | 403 |
| 1978 | Oct | 424 | 127.1 | 325 |
| 1978 | Nov | 505 | 117 | 373 |
| 1978 | Dec | 45 | 105.4 | 137 |

